Electronic supplementary information

# A Terminal Nickel(II) Anilide Complex Featuring an Unsymmetrically Substituted Amido Pincer Ligand: Synthesis and Reactivity

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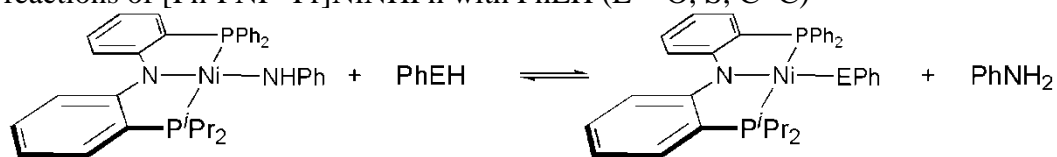- **Table S6.** Optimized coordinates of [Ph-PNP-$^i$Pr]NiC≡CPh

**Table S1.** Structures and selected bond distances (Å) and angles (deg) of DFT geometry optimized [Ph-PNP-$^i$Pr]NiEPh (E = NH, O, S, C≡C)
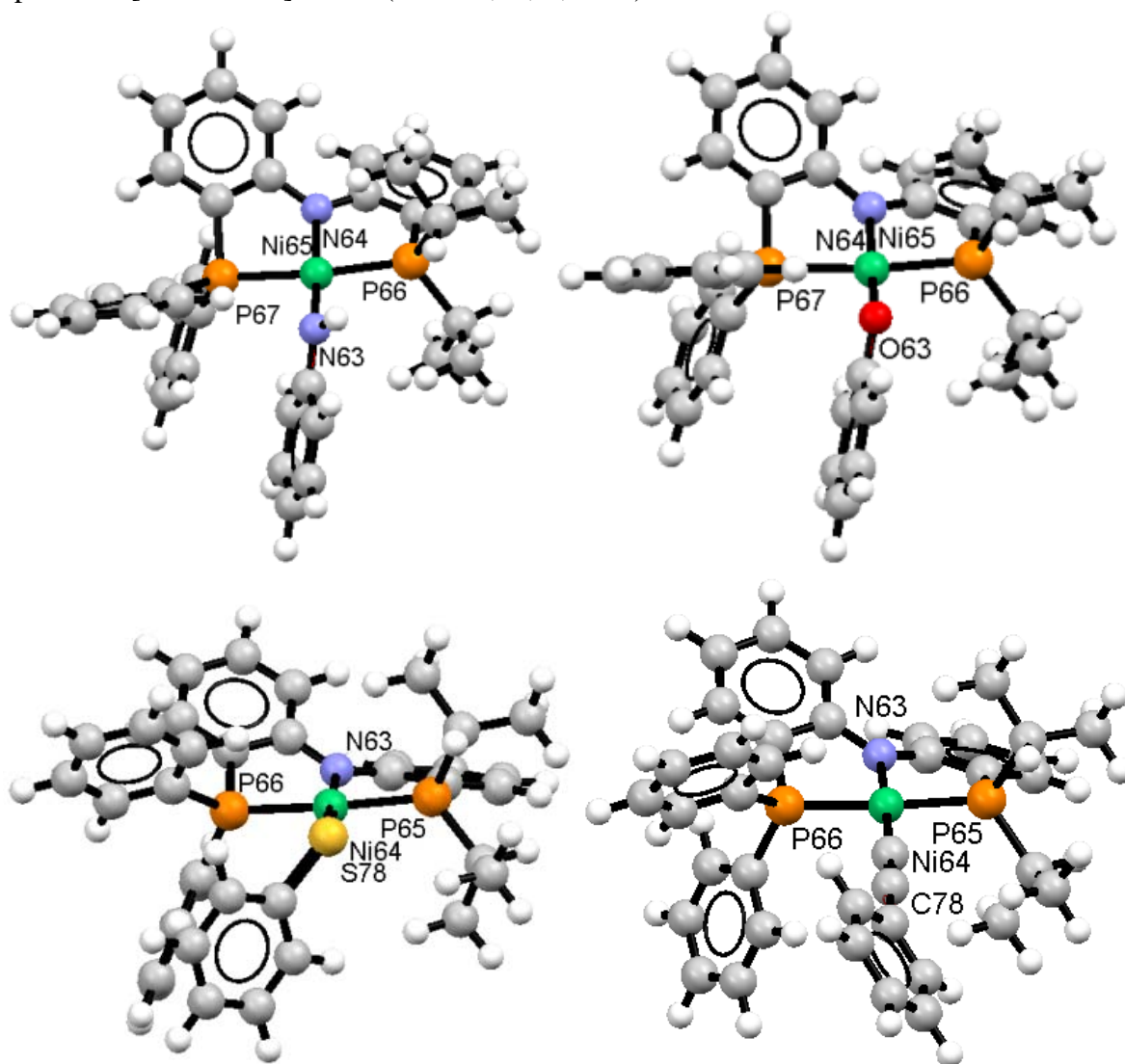


| E | NH | O | S | C≡C |
|---|---|---|---|---|
| Ni-X | 1.880 | 1.850 | 2.295 | 1.865 |
| N-Ni | 1.942 | 1.931 | 1.952 | 1.946 |
| Ph$_2$P-Ni | 2.362 | 2.326 | 2.313 | 2.253 |
| $^i$Pr$_2$P-Ni | 2.268 | 2.279 | 2.283 | 2.257 |
| ∠N-Ni-PPh$_2$ | 82.71 | 83.98 | 84.26 | 85.28 |
| ∠N-Ni-P$^i$Pr$_2$ | 85.24 | 85.07 | 84.98 | 85.88 |
| ∠Ph$_2$P-Ni-P$^i$Pr$_2$ | 166.12 | 168.83 | 169.13 | 170.97 |
| ∠N-Ni-X | 172.03 | 171.19 | 171.77 | 178.65 |
| ∠Ph$_2$P-Ni-X | 98.00 | 97.81 | 99.30 | 93.41 |
| ∠$^i$Pr$_2$P-Ni-X | 94.88 | 93.34 | 91.56 | 95.42 |

X represents the donor atom in E.

**Table S2.** DFT computed energy, enthalpy, and Gibbs free energy changes of exchange reactions of [Ph-PNP-$^i$Pr]NiNHPh with PhEH (E = O, S, C≡C)



| E | ΔE (kcal/mol) | ΔH (kcal/mol) | ΔG (kcal/mol) |
|---|---|---|---|
| O | -10.16 | -10.16 | -10.30 |
| S | -17.94 | -17.94 | -18.19 |
| C≡C | -6.11 | -6.11 | -7.23 |
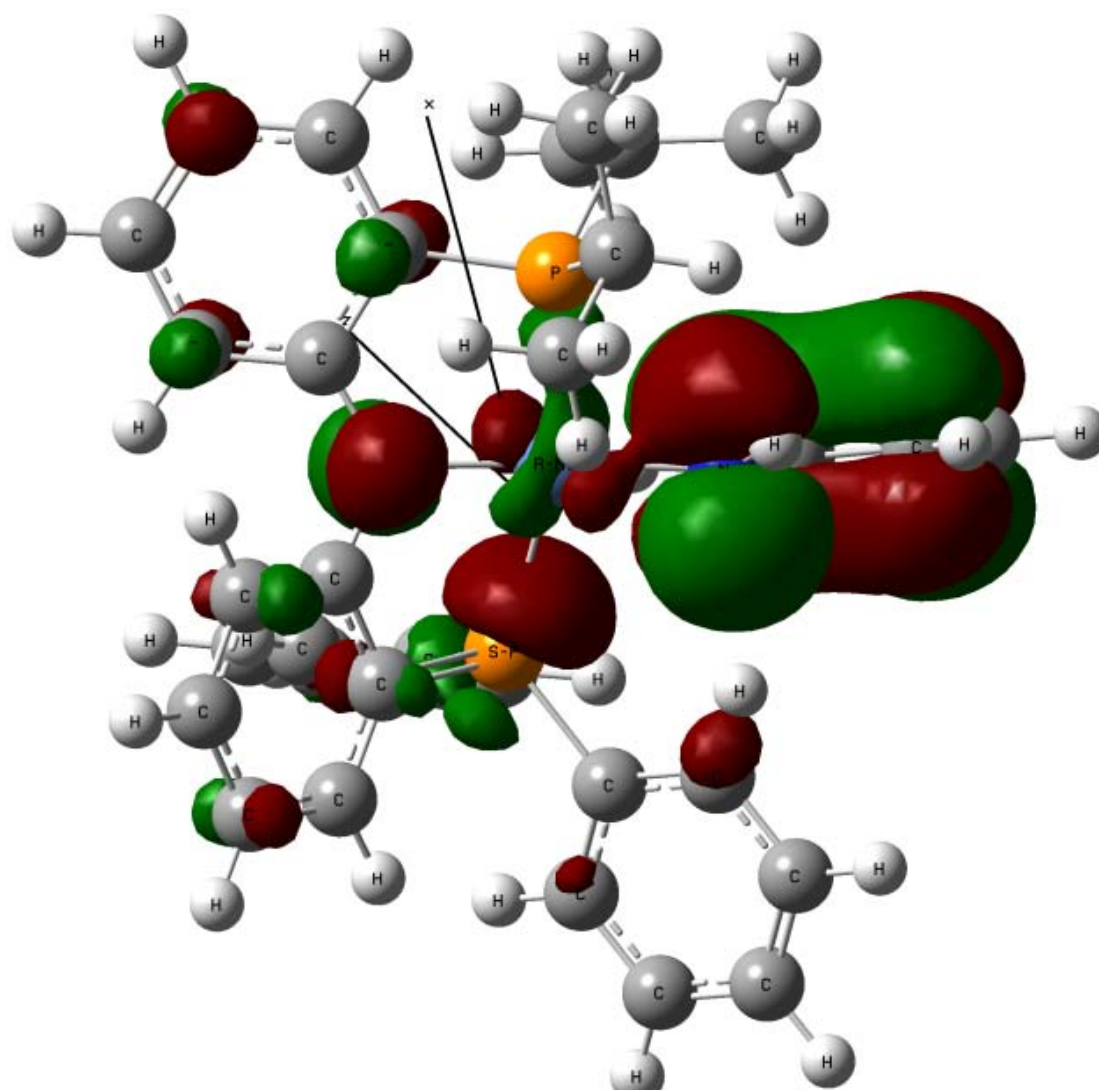
**Figure S1.** Contour plot of HOMO of [Ph-PNP-$^{i}$Pr]NiNHPh

**Table S3.** Optimized coordinates of [Ph-PNP-$^i$Pr]NiNHPh

| | | | |
|---|---|---|---|
| C | 0.40660000 | -2.54680000 | -0.63470000 |
| C | -0.99740000 | -2.37360000 | -0.74970000 |
| C | -1.81220000 | -3.35410000 | -1.31430000 |
| H | -2.88110000 | -3.17900000 | -1.39590000 |
| C | -1.26280000 | -4.54400000 | -1.79230000 |
| H | -1.89620000 | -5.30460000 | -2.23740000 |
| C | 0.12070000 | -4.72450000 | -1.70570000 |
| H | 0.57260000 | -5.63250000 | -2.09720000 |
| C | 0.94420000 | -3.75270000 | -1.14530000 |
| H | 2.01610000 | -3.91140000 | -1.12200000 |
| C | 2.40620000 | -1.71750000 | 0.47800000 |
| C | 3.34600000 | -0.65190000 | 0.48520000 |
| C | 4.60010000 | -0.78990000 | 1.08590000 |
| H | 5.29450000 | 0.04610000 | 1.08510000 |
| C | 4.96690000 | -1.98430000 | 1.70480000 |
| H | 5.93970000 | -2.08740000 | 2.17460000 |
| C | 4.04440000 | -3.03570000 | 1.72580000 |
| H | 4.29820000 | -3.96570000 | 2.22830000 |
| C | 2.79260000 | -2.91280000 | 1.13370000 |
| H | 2.09110000 | -3.73680000 | 1.19380000 |
| C | -3.07470000 | -0.26320000 | -1.16540000 |
| C | -2.89810000 | 0.64510000 | -2.21690000 |
| H | -1.92580000 | 1.10750000 | -2.35520000 |
| C | -3.97640000 | 0.97660000 | -3.03970000 |
| H | -3.83590000 | 1.68730000 | -3.84920000 |
| C | -5.23190000 | 0.40930000 | -2.81740000 |
| H | -6.06940000 | 0.67090000 | -3.45810000 |
| C | -5.41360000 | -0.48770000 | -1.76240000 |
| H | -6.39090000 | -0.92570000 | -1.58000000 |
| C | -4.34020000 | -0.82250000 | -0.93600000 |
| H | -4.49050000 | -1.50820000 | -0.10770000 |
| C | -2.30190000 | -1.06810000 | 1.57820000 |
| C | -3.14570000 | -0.12730000 | 2.18630000 |
| H | -3.41850000 | 0.78130000 | 1.65830000 |
| C | -3.63620000 | -0.35300000 | 3.47270000 |
| H | -4.29450000 | 0.37910000 | 3.93190000 |
| C | -3.28130000 | -1.51140000 | 4.16770000 |
| H | -3.66110000 | -1.68360000 | 5.17070000 |
| C | -2.43620000 | -2.44590000 | 3.56810000 |
| H | -2.15720000 | -3.35060000 | 4.10110000 |
| C | -1.94880000 | -2.22820000 | 2.27760000 |
| H | -1.30250000 | -2.96510000 | 1.81170000 |
| C | 3.26880000 | 2.34120000 | 0.80370000 |
| H | 4.35020000 | 2.20640000 | 0.93000000 |
| C | 2.59240000 | 2.23550000 | 2.17660000 |
| H | 2.98910000 | 3.01200000 | 2.84050000 |
| H | 2.77570000 | 1.26480000 | 2.64600000 |
| H | 1.51190000 | 2.38490000 | 2.09340000 |

| | | | |
|---|---|---|---|
| C | 3.00980000 | 3.70120000 | 0.14380000 |
| H | 1.94140000 | 3.86630000 | -0.01860000 |
| H | 3.52950000 | 3.80720000 | -0.81390000 |
| H | 3.37290000 | 4.49790000 | 0.80260000 |
| C | 3.60550000 | 1.10950000 | -1.98820000 |
| H | 3.18810000 | 2.03900000 | -2.39520000 |
| C | 3.22680000 | -0.05060000 | -2.91740000 |
| H | 3.67070000 | 0.10480000 | -3.90720000 |
| H | 2.14330000 | -0.13960000 | -3.03620000 |
| H | 3.60020000 | -1.00250000 | -2.52670000 |
| C | 5.12520000 | 1.25680000 | -1.85430000 |
| H | 5.56800000 | 0.35810000 | -1.41380000 |
| H | 5.41210000 | 2.11760000 | -1.24260000 |
| H | 5.57140000 | 1.39450000 | -2.84610000 |
| N | -0.08580000 | 2.00310000 | -0.93090000 |
| N | 1.16080000 | -1.50320000 | -0.10050000 |
| Ni | 0.51710000 | 0.30590000 | -0.39290000 |
| P | 2.70500000 | 0.89610000 | -0.30880000 |
| P | -1.59220000 | -0.72310000 | -0.12640000 |
| H | 0.42010000 | 2.40840000 | -1.71250000 |
| C | -0.71140000 | 2.97480000 | -0.18800000 |
| C | -0.91290000 | 4.28540000 | -0.69960000 |
| C | -1.21180000 | 2.71560000 | 1.11350000 |
| C | -1.59740000 | 5.25100000 | 0.02990000 |
| H | -0.53630000 | 4.52380000 | -1.69310000 |
| C | -1.89820000 | 3.69310000 | 1.83200000 |
| H | -1.03030000 | 1.74260000 | 1.55860000 |
| C | -2.10500000 | 4.96920000 | 1.30310000 |
| H | -1.73650000 | 6.23930000 | -0.40250000 |
| H | -2.26360000 | 3.45330000 | 2.82820000 |
| H | -2.63510000 | 5.72800000 | 1.87020000 |

**Table S4.** Optimized coordinates of [Ph-PNP-$^i$Pr]NiOPh

| | | | |
|---|---|---|---|
| C | 0.42164600 | -2.56616800 | -0.49998800 |
| C | -0.98196800 | -2.40602500 | -0.64339600 |
| C | -1.78646800 | -3.41463300 | -1.17295300 |
| H | -2.85468300 | -3.24653800 | -1.27671900 |
| C | -1.22718800 | -4.62220400 | -1.58956700 |
| H | -1.85144300 | -5.40520500 | -2.00775200 |
| C | 0.15656300 | -4.78997500 | -1.47903000 |
| H | 0.61774600 | -5.71161000 | -1.82518700 |
| C | 0.96954000 | -3.79122500 | -0.95258100 |
| H | 2.04124100 | -3.94540900 | -0.91004400 |
| C | 2.42867900 | -1.68356200 | 0.56477800 |
| C | 3.36625800 | -0.61956400 | 0.49625100 |
| C | 4.63740100 | -0.73448200 | 1.06411900 |
| H | 5.33322400 | 0.09801700 | 1.00118300 |
| C | 5.01957200 | -1.90010400 | 1.72791000 |
| H | 6.00645400 | -1.98495600 | 2.17137100 |
| C | 4.09595700 | -2.94501800 | 1.82911600 |
| H | 4.36153300 | -3.84988500 | 2.36980700 |
| C | 2.82705800 | -2.84536500 | 1.26807100 |
| H | 2.12381600 | -3.66114500 | 1.38959100 |
| C | -2.97785400 | -0.24926400 | -1.26308400 |
| C | -2.70078900 | 0.63868000 | -2.31106900 |
| H | -1.71241000 | 1.08103600 | -2.38811600 |
| C | -3.70851300 | 0.97983400 | -3.21557100 |
| H | -3.49184600 | 1.67344800 | -4.02291100 |
| C | -4.99040200 | 0.44584300 | -3.07686200 |
| H | -5.77209300 | 0.71638300 | -3.78111500 |
| C | -5.27171300 | -0.42723300 | -2.02357500 |
| H | -6.27087600 | -0.83703400 | -1.90583700 |
| C | -4.27019500 | -0.77318000 | -1.11598200 |
| H | -4.49789800 | -1.43938900 | -0.28927600 |
| C | -2.41065200 | -0.98797700 | 1.55376200 |
| C | -2.19650200 | -2.16319800 | 2.28267100 |
| H | -1.58620200 | -2.95592900 | 1.86209700 |
| C | -2.77487300 | -2.32019000 | 3.54427300 |
| H | -2.60517300 | -3.23675600 | 4.10219900 |
| C | -3.57016900 | -1.30832000 | 4.08308000 |
| H | -4.02049500 | -1.43272900 | 5.06377200 |
| C | -3.78352200 | -0.13337800 | 3.35819300 |
| H | -4.39977100 | 0.65955200 | 3.77226100 |
| C | -3.20338900 | 0.03130500 | 2.10037400 |
| H | -3.36159200 | 0.95407300 | 1.55103500 |
| C | 3.34961500 | 2.39908000 | 0.63625700 |
| H | 4.43992500 | 2.27493100 | 0.65724100 |
| C | 2.82284600 | 2.37969500 | 2.07669700 |
| H | 3.29033300 | 3.19038400 | 2.64720400 |
| H | 3.05086000 | 1.43708500 | 2.58249500 |
| H | 1.74035500 | 2.53540100 | 2.10001100 |

| | | | |
|---|---|---|---|
| C | 3.01208000 | 3.71446100 | -0.07849800 |
| H | 1.93178600 | 3.85338200 | -0.16990200 |
| H | 3.45121300 | 3.76870400 | -1.07931400 |
| H | 3.41292900 | 4.55334400 | 0.50159300 |
| C | 3.45558000 | 1.00116700 | -2.08472200 |
| H | 3.01309000 | 1.91315300 | -2.50181200 |
| C | 2.99082100 | -0.19632000 | -2.92225600 |
| H | 3.36602400 | -0.09986600 | -3.94739700 |
| H | 1.90007200 | -0.26182600 | -2.96118600 |
| H | 3.37143400 | -1.13746700 | -2.51226300 |
| C | 4.98207800 | 1.13071300 | -2.06929300 |
| H | 5.44665100 | 0.24707800 | -1.61991300 |
| H | 5.32176700 | 2.01457700 | -1.52076100 |
| H | 5.35657200 | 1.21700600 | -3.09594400 |
| O | -0.08874600 | 1.94668800 | -0.86786800 |
| N | 1.16508600 | -1.50070300 | 0.00452800 |
| Ni | 0.49293300 | 0.28389100 | -0.30133300 |
| P | 2.68859100 | 0.89344000 | -0.33255700 |
| P | -1.59078600 | -0.73285200 | -0.11318800 |
| C | -0.70414900 | 2.85455100 | -0.11613200 |
| C | -1.10969300 | 4.07161300 | -0.71723300 |
| C | -0.97201700 | 2.68646000 | 1.26238700 |
| C | -1.75213700 | 5.05708000 | 0.02544800 |
| H | -0.90691200 | 4.21175900 | -1.77526600 |
| C | -1.61675400 | 3.68577400 | 1.99539800 |
| H | -0.66733000 | 1.76236800 | 1.74654800 |
| C | -2.01351400 | 4.87802600 | 1.38901700 |
| H | -2.05297300 | 5.97932600 | -0.46634100 |
| H | -1.80651800 | 3.52457200 | 3.05425400 |
| H | -2.51305600 | 5.65245000 | 1.96308400 |

**Table S5.** Optimized coordinates of [Ph-PNP-$^i$Pr]NiSPh

| | | | |
|---|---|---|---|
| C | -0.89799900 | 2.53607700 | -0.23741500 |
| C | 0.51397200 | 2.55945700 | -0.35974800 |
| C | 1.20384700 | 3.71349600 | -0.73147500 |
| H | 2.28644800 | 3.68279700 | -0.81752500 |
| C | 0.51380700 | 4.89056300 | -1.01615200 |
| H | 1.04836500 | 5.78811800 | -1.31000600 |
| C | -0.88292700 | 4.87714600 | -0.94483400 |
| H | -1.44512800 | 5.77199300 | -1.20022700 |
| C | -1.57998800 | 3.73317000 | -0.57114600 |
| H | -2.66298500 | 3.75391900 | -0.55406200 |
| C | -2.79791700 | 1.32823900 | 0.67299100 |
| C | -3.60137100 | 0.17235800 | 0.49817500 |
| C | -4.89289300 | 0.09756800 | 1.02658600 |
| H | -5.48566300 | -0.80084300 | 0.87767200 |
| C | -5.42681200 | 1.15482500 | 1.76210900 |
| H | -6.42951500 | 1.09205800 | 2.17250500 |
| C | -4.62961000 | 2.28225500 | 1.98281200 |
| H | -5.00903400 | 3.10241100 | 2.58711400 |
| C | -3.34434600 | 2.37193900 | 1.46018500 |
| H | -2.74290300 | 3.24760900 | 1.67367900 |
| C | 2.70035200 | 0.83611500 | -1.33073400 |
| C | 2.41289900 | 0.33078200 | -2.60551700 |
| H | 1.43221600 | -0.08720400 | -2.80617400 |
| C | 3.39566800 | 0.33215100 | -3.59632100 |
| H | 3.16562100 | -0.06458400 | -4.58102800 |
| C | 4.67078900 | 0.83060800 | -3.32083200 |
| H | 5.43553400 | 0.82724500 | -4.09238800 |
| C | 4.96177800 | 1.32914000 | -2.05014300 |
| H | 5.95253500 | 1.71596900 | -1.82897900 |
| C | 3.98037700 | 1.33443900 | -1.05661300 |
| H | 4.21535900 | 1.71987600 | -0.06969000 |
| C | 2.15486500 | 1.01452100 | 1.59864800 |
| C | 1.76937300 | 1.99842600 | 2.51748200 |
| H | 1.02319100 | 2.73558800 | 2.23878200 |
| C | 2.35077600 | 2.03807400 | 3.78604600 |
| H | 2.04805500 | 2.80660800 | 4.49164600 |
| C | 3.31936800 | 1.09899600 | 4.14398200 |
| H | 3.77239700 | 1.13252200 | 5.13081500 |
| C | 3.70289300 | 0.11555000 | 3.22997100 |
| H | 4.45267600 | -0.62206300 | 3.50076100 |
| C | 3.12094100 | 0.06632400 | 1.96263400 |
| H | 3.42313400 | -0.70680500 | 1.26435300 |
| C | -3.20264900 | -2.77552600 | 0.62643100 |
| H | -4.29414300 | -2.72497200 | 0.72355700 |
| C | -2.58489600 | -2.69462300 | 2.02740100 |
| H | -2.90371100 | -3.55735100 | 2.62331700 |
| H | -2.89094600 | -1.78666400 | 2.55477900 |
| H | -1.49267100 | -2.70672100 | 1.96986700 |

| | | | |
|---|---|---|---|
| C | -2.82650100 | -4.07407900 | -0.09628200 |
| H | -1.74892300 | -4.12948200 | -0.27036200 |
| H | -3.33270300 | -4.17336700 | -1.06148600 |
| H | -3.12654200 | -4.92880200 | 0.52113200 |
| C | -3.46880700 | -1.41799200 | -2.11872700 |
| H | -2.93213000 | -2.28374200 | -2.52409500 |
| C | -3.12593300 | -0.18650100 | -2.96576500 |
| H | -3.48607200 | -0.32899100 | -3.99091000 |
| H | -2.04696400 | -0.01360300 | -3.00284400 |
| H | -3.60090900 | 0.71483400 | -2.56454500 |
| C | -4.97416100 | -1.70544100 | -2.11173900 |
| H | -5.53367700 | -0.86368200 | -1.69115200 |
| H | -5.22788700 | -2.60532500 | -1.54306200 |
| H | -5.32514300 | -1.85634900 | -3.13928700 |
| N | -1.51490800 | 1.34298400 | 0.13063900 |
| Ni | -0.61701400 | -0.33608100 | -0.29787400 |
| P | -2.72341100 | -1.21254100 | -0.36762800 |
| P | 1.31789900 | 0.91039200 | -0.07372900 |
| C | 1.79178500 | -2.74562800 | -0.14971300 |
| C | 3.03500500 | -2.79932500 | -0.79762000 |
| C | 1.71316100 | -3.14721600 | 1.19217500 |
| C | 4.17021200 | -3.24730800 | -0.11768600 |
| H | 3.10699800 | -2.49099400 | -1.83492600 |
| C | 2.84956500 | -3.59015100 | 1.87019000 |
| H | 0.75595400 | -3.12006200 | 1.70189100 |
| C | 4.08432900 | -3.64379800 | 1.21888400 |
| H | 5.12408700 | -3.28531100 | -0.63729700 |
| H | 2.76694000 | -3.89855600 | 2.90910600 |
| H | 4.96744700 | -3.99592100 | 1.74456200 |
| S | 0.28940100 | -2.28789700 | -1.09428500 |

**Table S6.** Optimized coordinates of [Ph-PNP-$^i$Pr]NiC≡CPh

| | | | |
|---|---|---|---|
| C | 2.16281600 | -1.96583200 | -0.66283800 |
| C | 0.95013200 | -2.70649800 | -0.62134700 |
| C | 0.86318100 | -4.01338800 | -1.10156700 |
| H | -0.09171500 | -4.53173900 | -1.06946500 |
| C | 1.98147600 | -4.64297900 | -1.64741500 |
| H | 1.91643100 | -5.65864400 | -2.02404400 |
| C | 3.17602700 | -3.92108000 | -1.73006000 |
| H | 4.04999000 | -4.37616300 | -2.18951800 |
| C | 3.27206000 | -2.61534600 | -1.25888700 |
| H | 4.20449800 | -2.07713600 | -1.37861200 |
| C | 3.31796500 | -0.01299200 | 0.22999600 |
| C | 3.34273700 | 1.40893100 | 0.25502100 |
| C | 4.46898000 | 2.11090800 | 0.69033600 |
| H | 4.45492600 | 3.19749600 | 0.70046500 |
| C | 5.60499800 | 1.43636300 | 1.13724100 |
| H | 6.47634100 | 1.98558300 | 1.47909700 |
| C | 5.57945000 | 0.03917900 | 1.16423400 |
| H | 6.43630400 | -0.50935800 | 1.54745800 |
| C | 4.46750900 | -0.67421300 | 0.72928600 |
| H | 4.47207000 | -1.75491800 | 0.80124800 |
| C | -1.96715600 | -2.20084500 | -1.00947000 |
| C | -2.23488900 | -1.49091300 | -2.18671300 |
| H | -1.61225300 | -0.64369600 | -2.45541000 |
| C | -3.31049200 | -1.85914200 | -2.99554000 |
| H | -3.51262900 | -1.30470700 | -3.90755200 |
| C | -4.12997800 | -2.92944900 | -2.62879600 |
| H | -4.97037600 | -3.21122300 | -3.25676400 |
| C | -3.87225600 | -3.63104300 | -1.45031700 |
| H | -4.51095500 | -4.45943900 | -1.15736300 |
| C | -2.79367400 | -3.26864300 | -0.64049000 |
| H | -2.60237100 | -3.81091900 | 0.28055600 |
| C | -0.87941500 | -2.26830400 | 1.74951500 |
| C | -0.34013400 | -3.43575900 | 2.30047000 |
| H | 0.33506400 | -4.05047700 | 1.71323200 |
| C | -0.66531300 | -3.80351800 | 3.60857100 |
| H | -0.24387400 | -4.71043200 | 4.03290400 |
| C | -1.52534500 | -3.00840000 | 4.36718200 |
| H | -1.77573600 | -3.29571700 | 5.38447700 |
| C | -2.05767600 | -1.83803400 | 3.81990000 |
| H | -2.72023200 | -1.21195000 | 4.41065400 |
| C | -1.73433600 | -1.46306700 | 2.51606100 |
| H | -2.13043000 | -0.54373200 | 2.09346100 |
| C | 1.43206300 | 3.61247000 | 0.99768300 |
| H | 2.37157300 | 4.17737100 | 1.04006800 |
| C | 1.14103300 | 3.02251100 | 2.38354400 |
| H | 1.03530000 | 3.83142500 | 3.11559300 |
| H | 1.94636900 | 2.36398900 | 2.72214300 |
| H | 0.20933500 | 2.44931000 | 2.36732400 |

| | | | |
|---|---|---|---|
| C | 0.30633100 | 4.54124900 | 0.52541600 |
| H | -0.62484800 | 3.98503800 | 0.38817000 |
| H | 0.54789800 | 5.04566800 | -0.41509900 |
| H | 0.13657000 | 5.31829600 | 1.27964700 |
| C | 1.95471300 | 2.98529500 | -1.96290600 |
| H | 0.97929100 | 3.44316300 | -2.16333600 |
| C | 2.20514500 | 1.88590600 | -3.00217100 |
| H | 2.26401700 | 2.32739400 | -4.00351500 |
| H | 1.40393300 | 1.14199700 | -3.00066000 |
| H | 3.14892600 | 1.36644700 | -2.80699400 |
| C | 3.04449400 | 4.06251400 | -2.00015200 |
| H | 4.02745400 | 3.63469300 | -1.77888700 |
| H | 2.85700400 | 4.87570500 | -1.29196300 |
| H | 3.09310100 | 4.50391800 | -3.00250400 |
| N | 2.15661600 | -0.65094500 | -0.20087000 |
| Ni | 0.47111400 | 0.31959000 | -0.14401600 |
| P | 1.73206900 | 2.18974800 | -0.23671500 |
| P | -0.48203500 | -1.71648600 | 0.00985000 |
| C | -3.55729300 | 2.36636900 | 0.02083300 |
| C | -4.58505300 | 1.95209200 | -0.85304600 |
| C | -3.84022900 | 3.40184300 | 0.93660300 |
| C | -5.83931500 | 2.55601700 | -0.81425600 |
| H | -4.38227300 | 1.14969000 | -1.55540500 |
| C | -5.09812300 | 3.99914500 | 0.97213100 |
| H | -3.06074700 | 3.72719600 | 1.61876000 |
| C | -6.10365100 | 3.58216600 | 0.09661900 |
| H | -6.61626800 | 2.22268400 | -1.49715800 |
| H | -5.29434000 | 4.79495100 | 1.68579100 |
| H | -7.08331000 | 4.05059800 | 0.12492200 |
| C | -1.16416100 | 1.21293000 | -0.07572600 |
| C | -2.26796200 | 1.75135700 | -0.02398400 |