

Supporting Information for

Origins of the Selectivity of Late Transition Metals of Group 9 and Group 10 for Oxidative Addition of C–H vs C–Cl Bonds

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1. Computational Methods

All calculations were performed with the Q-Chem (Version 5.4.1) program.^[1] Geometry optimizations were conducted with the PBE0 functional^[2] and the basis sets def2-SVP for H atoms, def2-SVPD for O, Cl, and P atoms, and def2-TZVP (with matching Karlsruhe effective core potential, def2-ECP) for metal centers (**BS1**),^[3] with Grimme's D3 dispersion correction with Becke-Johnson damping (D3BJ)^[4] in the gas phase. The nature of each stationary point was evaluated by accompanying frequency calculations (all positive eigenvalues for ground states and precisely one negative eigenvalue for transition states). Further single-point energy calculations were performed on the optimized structures with the def2-TZVPD basis set (with def2-ECP for metal centers) for all atoms (**BS2**) using the SMD solvation model with chlorobenzene as the solvent. In all cases, Gibbs free energies for **BS2** were estimated by adding the thermal corrections obtained from frequency calculations using **BS1** to the electronic energies computed at **BS2**.

Energy decomposition analysis was performed using the second-generation absolutely localized molecular orbital energy decomposition analysis (ALMO-EDA).^[5] Natural Bond Orbital (NBO) and Natural Population Analysis (NPA) were conducted with the NBO 5.0 program.^[6] AIM calculations were conducted with the Multiwfn (Version 3.8) program.^[7]

Literature suggests that the PBE0 functional performs well for Pd-mediated bond activation reactions and for calculating barriers to a broad set of transition-metal-mediated insertion and bond activation reactions.^[8-11] Nevertheless, computed energy differences on the order of 1–3 kcal/mol lie near the expected uncertainty of DFT methods for these systems and should be interpreted qualitatively in the context of experimental observations and other computational data.

2. Distortion/Interaction Model and Energy Decomposition Analysis

The Activation Strain Model (ASM)^[12-14] or the Distortion/Interaction Model^[15-16] decomposes the potential energy surface $\Delta E(\zeta)$ along the reaction coordinate ζ of a given chemical reaction into two terms: the reaction strain or distortion energy, $\Delta E_{\text{strain}}(\zeta)$, and the interaction energy, $\Delta E_{\text{int}}(\zeta)$; ^[17] that is,

$$\Delta E(\zeta) = \Delta E_{\text{strain}}(\zeta) + \Delta E_{\text{int}}(\zeta) \quad (\text{S1})$$

The distortion energy, $\Delta E_{\text{strain}}(\zeta)$, refers to the energy required to distort the geometries of the reactants from their lowest-energy ground states to the reactive conformations. By definition, the distortion energy is destabilizing, *i.e.*, $\Delta E_{\text{strain}}(\zeta) > 0$. The interaction energy, $\Delta E_{\text{int}}(\zeta)$, refers to the change in energy caused by interactions between the distorted reactive fragments and is stabilizing, *i.e.*, $\Delta E_{\text{int}}(\zeta) < 0$. Therefore, the sum of $\Delta E_{\text{strain}}(\zeta)$ and $\Delta E_{\text{int}}(\zeta)$ determines the energy profile of a chemical reaction along the reaction coordinate. At the transition state, the potential energy surface reaches a first-order saddle point; that is, for $\zeta = \zeta(\text{TS})$,

$$\frac{\partial \Delta E(\zeta)}{\partial \zeta} = \frac{\partial \Delta E_{\text{strain}}(\zeta)}{\partial \zeta} + \frac{\partial \Delta E_{\text{int}}(\zeta)}{\partial \zeta} = 0 \quad (\text{S2})$$

Rearrangement of eq S2 gives the following equation:

$$\frac{\partial \Delta E_{\text{strain}}(\zeta)}{\partial \zeta} = - \frac{\partial \Delta E_{\text{int}}(\zeta)}{\partial \zeta} \quad (\text{S3})$$

This equation shows that the rate by which $\Delta E_{\text{strain}}(\zeta)$ increases is equal to the rate by which $\Delta E_{\text{int}}(\zeta)$ decreases at the transition state.

According to Energy Decomposition Analysis based on Absolutely Localized Molecular Orbitals (ALMO EDA),^[18-20] the interaction energy, ΔE_{int} , can be further decomposed into three terms: the frozen density term (ΔE_{FRZ}), the polarization term, (ΔE_{POL}), and the charge transfer term, (ΔE_{CT}). The frozen density term (ΔE_{FRZ}) is defined as the change in energy caused by bringing infinitely separated, distorted reactive fragments into the reactive complex without any relaxation of the molecular orbitals (MOs) on those fragments and describes primarily the Pauli repulsion, permanent electrostatic interaction and dispersion of the reactants. The polarization term (ΔE_{POL}) refers to the stabilization energy attributable to relaxation of localized MOs on each reactive fragment in the field produced by all other fragments and quantifies the polarization of electron density that is induced by the approaching reactive fragments. Lastly, the charge transfer term (ΔE_{CT}) describes the stabilization caused by charge transfer from occupied orbitals of one reactive fragment to virtual orbitals of another fragment. ALMO EDA allows the interaction energy (ΔE_{int}) to be interpreted in chemically meaningful terms, such as electrostatic interactions and orbital interactions,^[20] and has been used for the analysis of many chemical systems.^[18-25]

3. Oxidative Addition of *ortho*- versus *para*-C–H bond in PhCl to (L1)Ir and (L1)Rh Complexes

Consistent with published experimental^[26-27] and computational^[28-29] studies, our calculations suggest that oxidative addition of the *ortho*-C–H bond in PhCl to (L1)Ir and (L1)Rh complexes is more favorable than that of the *para*-C–H bond (see Figures S1 and S2) because during the reaction with the *ortho*-C–H bond, the proximal chlorine atom partially coordinates to the metal center and stabilizes the transition state and the product whereas such stabilization is absent in the reaction with the *para*-C–H bond due to the long distance between Cl and the metal center. Although the reaction with the *para*-C–H bond is less energetically favorable than that with the *ortho*-C–H bond, we still chose the former as the model system so that our analysis can focus on the interactions between the metal complex and the C–H bond, without interfering interactions between Cl and the metal center.

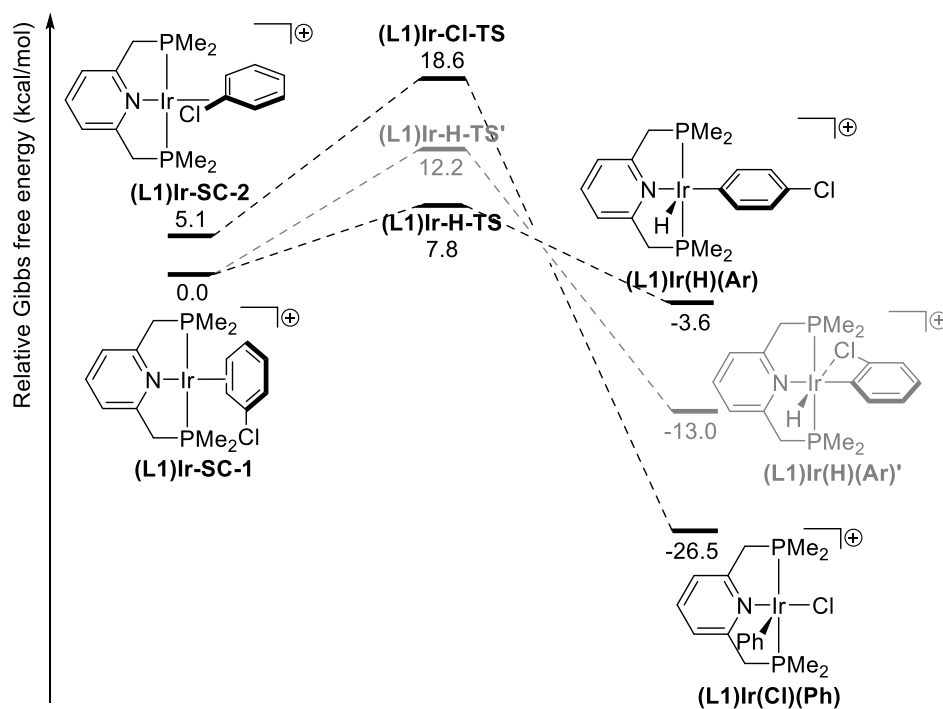


Figure S1. Free-energy diagram of the oxidative addition of the *ortho*- and *para*-C–H bonds as well as the C–Cl bond in PhCl to (L1)Ir(I) complexes.

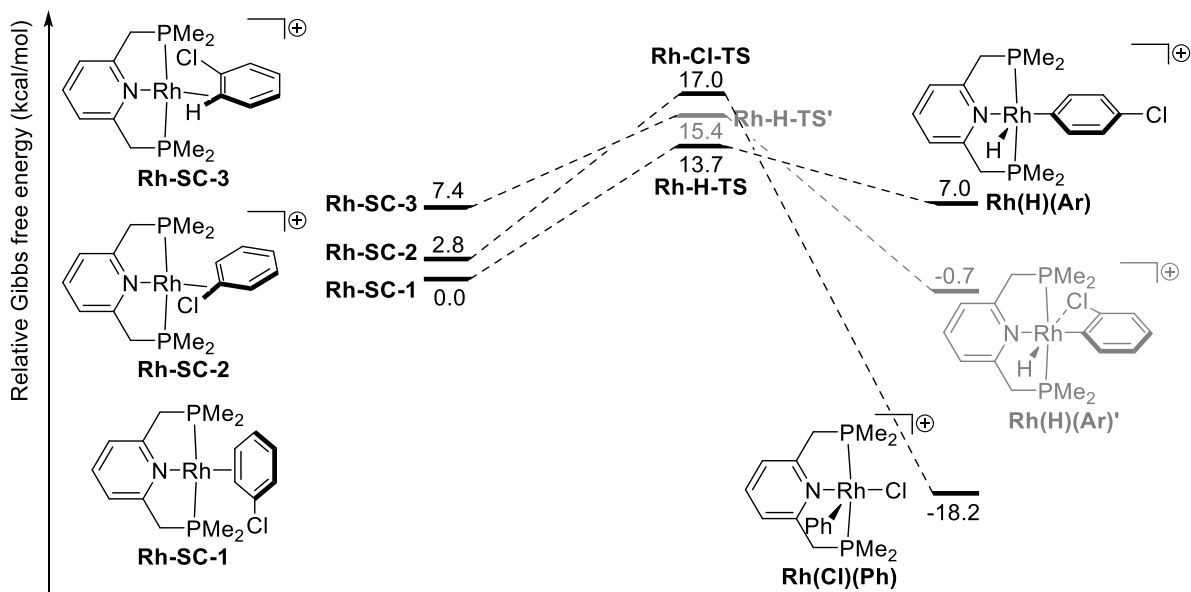


Figure S2. Free-energy diagram of the oxidative addition of the *ortho*- and *para*-C–H bonds as well as the C–Cl bond in PhCl to (L1)Rh(I) complexes.

4. Oxidative Addition of Aryl C–H and C–Cl Bonds to (tBuL1)Ir and (tBuL1)Rh Complexes

To investigate the steric effect of the ligand on the selectivity of oxidative addition, we calculated Ir and Rh complexes containing the ligand, 2,6-bis((di-*tert*-butylphosphino)methyl)pyridine (**tBuL1**), which is more sterically demanding than the ligand **L1** containing methyl groups on phosphorus. The results are shown in Figures S3 and S4. For (**L1**)Rh and (**L1**)Ir complexes, the π -complex between the C(2)–C(3) bond of the chlorobenzene and the metal center (**Ir-SC-1** or **Rh-SC-1**) is the lowest-energy structure prior to the transition state. For (**tBuL1**)Rh and (**tBuL1**)Ir complexes, however, the σ -complex between the C–Cl bond and the metal center (**Ir-SC-2** or **Rh-SC-2**) was found to be the lowest-energy structure prior to the transition state. We propose that steric interactions between PhCl and the *tert*-butyl substituents in (**tBuL1**)**Ir-SC-1** and (**tBuL1**)**Rh-SC-1** significantly destabilize these structures, whereas such interactions are negligible in (**tBuL1**)**Ir-SC-2** and (**tBuL1**)**Rh-SC-2** because the phenyl ring is positioned far away from the *tert*-butyl groups.

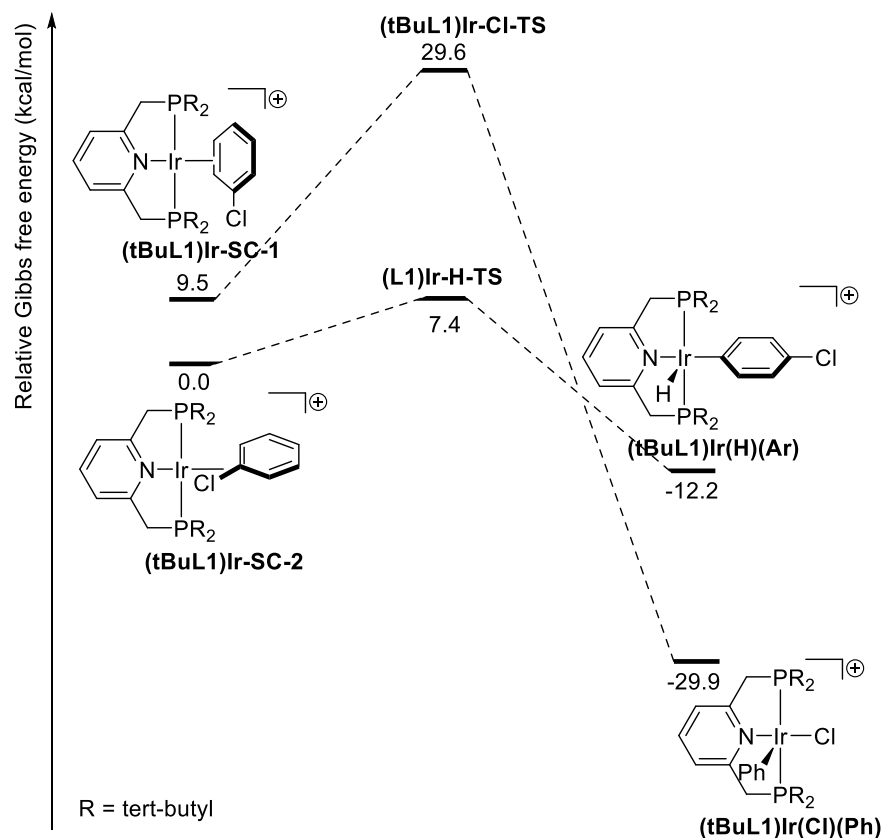


Figure S3. Free-energy diagram of the oxidative addition of the *ortho*-C–H bond and the C–Cl bond in PhCl to (**tBuL1**)Ir(I) complexes.

Oxidative addition of an aryl C–H bond to (**tBuL1**)M⁺ (M = Ir or Rh) is thermodynamically more favorable than that to the corresponding (**L1**)M⁺ complex, whereas the ΔG value for oxidative addition of an aryl C–Cl bond to (**L1**)M⁺ is similar to that for oxidative addition to

(**tBuL1**)M⁺. The barrier to oxidative addition of an aryl C–Cl bond to (**tBuL1**)M⁺ is significantly higher (by over 10 kcal/mol) than that to the corresponding (**L1**)M⁺ complex, whereas the barrier to oxidative addition of an aryl C–H bond to (**L1**)M⁺ is similar to that for addition to (**tBuL1**)M⁺. These computed data suggest that Group 9 metal complexes containing the bulky **tBuL1** ligand are more selective for the oxidative addition of aryl C–H bonds over aryl C–Cl bonds than those containing the **L1** ligand, and that products from C–H activation are the only products that will be formed when PhCl reacts with (**L1**)M⁺ or (**tBuL1**)M⁺. These conclusions are consistent with reported experimental results.^[26, 30]

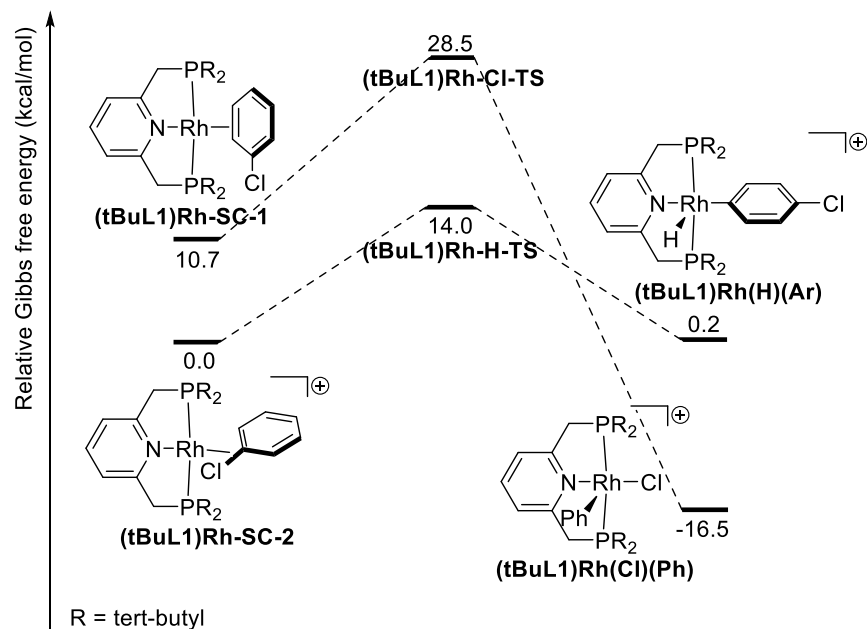


Figure S4. Free-energy diagram of the oxidative addition of the *ortho*-C–H bond and the C–Cl bond in PhCl to (**tBuL1**)Rh(I) complexes.

5. Energies of Optimized Structures

Table S1. Energies of Optimized Structures.

| Structure | E(BS1) (Hartree) | Thermal Correction | Thermal Correction | E(BS2) (Hartree) |
|-------------------|------------------|---------------------------|--|------------------|
| | | to Enthalpy (kcal/mol) | to Entropy (cal mol ⁻¹ K ⁻¹) | |
| PhCl | -691.129164 | 61.607 | 76.062 | -691.525282 |
| (L1)Ir-SC-1 | -1962.181526 | 251.223 | 165.752 | -1963.391189 |
| (L1)Ir-SC-2 | -1962.170445 | 251.463 | 172.489 | -1963.380206 |
| (L1)Ir-H-TS | -1962.157335 | 248.287 | 171.445 | -1963.371382 |
| (L1)Ir-H-TS' | -1962.158370 | 248.478 | 166.716 | -1963.366919 |
| (L1)Ir-Cl-TS | -1962.146672 | 250.201 | 167.072 | -1963.359270 |
| (L1)Ir(H)(Ar) | -1962.175185 | 249.188 | 172.899 | -1963.390307 |
| (L1)Ir(H)(Ar)' | -1962.201173 | 249.517 | 166.486 | -1963.408819 |
| (L1)Ir(Cl)(Ph) | -1962.222598 | 251.358 | 169.023 | -1963.432110 |
| (tBuL1)Ir-SC-1 | -2433.042523 | 472.378 | 216.834 | -2434.733940 |
| (tBuL1)Ir-SC-2 | -2433.051535 | 471.282 | 222.380 | -2434.744512 |
| (tBuL1)Ir-H-TS | -2433.034647 | 468.982 | 218.060 | -2434.729622 |
| (tBuL1)Ir-Cl-TS | -2433.011701 | 472.080 | 213.343 | -2434.704118 |
| (tBuL1)Ir(H)(Ar) | -2433.067677 | 469.771 | 219.489 | -2434.763988 |
| (tBuL1)Ir(Cl)(Ph) | -2433.104305 | 472.306 | 217.965 | -2434.792742 |
| (L3)Ir-SC-1 | -2153.151397 | 278.606 | 180.774 | -2154.518228 |
| (L3)Ir-H-TS | -2153.117016 | 277.339 | 181.896 | -2154.488068 |
| (L3)Ir-Cl-TS | -2153.109490 | 277.727 | 183.898 | -2154.483123 |
| (L3)Ir(H)(Ar) | -2153.149517 | 276.823 | 188.817 | -2154.517776 |
| (L3)Ir(Cl)(Ph) | -2153.201794 | 278.987 | 184.741 | -2154.564878 |
| Rh-SC-1 | -1968.379119 | 251.145 | 166.474 | -1969.587231 |
| Rh-SC-2 | -1968.373452 | 251.398 | 171.036 | -1969.581072 |
| Rh-SC-3 | -1968.366137 | 250.749 | 169.508 | -1969.573384 |
| Rh-H-TS | -1968.345644 | 248.103 | 170.792 | -1969.558572 |
| Rh-H-TS' | -1968.351146 | 248.173 | 167.493 | -1969.557481 |
| Rh-Cl-TS | -1968.346519 | 250.075 | 167.555 | -1969.557957 |
| Rh(H)(Ar) | -1968.355429 | 248.863 | 172.087 | -1969.569809 |
| Rh(H)(Ar)' | -1968.378926 | 249.191 | 166.770 | -1969.585106 |
| Rh(Cl)(Ph) | -1968.405346 | 251.238 | 168.352 | -1969.615421 |
| (tBuL1)Rh-SC-1 | -2439.241827 | 472.339 | 216.871 | -2440.933043 |
| (tBuL1)Rh-SC-2 | -2439.254160 | 471.414 | 221.053 | -2440.945183 |
| (tBuL1)Rh-H-TS | -2439.226933 | 469.189 | 216.613 | -2440.920996 |
| (tBuL1)Rh-Cl-TS | -2439.213208 | 471.750 | 214.167 | -2440.904360 |
| (tBuL1)Rh(H)(Ar) | -2439.246840 | 469.173 | 220.295 | -2440.942206 |
| (tBuL1)Rh(Cl)(Ph) | -2439.287183 | 472.770 | 215.302 | -2440.976254 |
| Pd-SC | -1864.760693 | 379.232 | 185.012 | -1866.018376 |
| Pd-H-TS | -1864.712937 | 376.132 | 187.779 | -1865.974077 |
| Pd-Cl-TS | -1864.739286 | 378.877 | 180.220 | -1865.998335 |
| Pd(H)(Ar) | -1864.713222 | 376.862 | 189.243 | -1865.975306 |

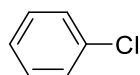
| | | | | |
|-------------------|--------------|---------|---------|--------------|
| Pd(Cl)(Ph) | -1864.776740 | 380.118 | 182.106 | -1866.043072 |
| Pt-SC | -1856.208349 | 379.190 | 188.052 | -1857.468860 |
| Pt-H-TS | -1856.178406 | 376.548 | 186.891 | -1857.439838 |
| Pt-Cl-TS | -1856.185409 | 379.160 | 181.569 | -1857.448425 |
| Pt(H)(Ar) | -1856.187422 | 377.478 | 190.508 | -1857.450664 |
| Pt(Cl)(Ph) | -1856.245618 | 380.247 | 182.265 | -1857.511305 |

6. References

- [1] E. Epifanovsky, A. T. B. Gilbert, X. Feng, J. Lee, Y. Mao, N. Mardirossian, P. Pokhilko, A. F. White, M. P. Coons, A. L. Dempwolff, Z. Gan, D. Hait, P. R. Horn, L. D. Jacobson, I. Kaliman, J. Kussmann, A. W. Lange, K. U. Lao, D. S. Levine, J. Liu, S. C. McKenzie, A. F. Morrison, K. D. Nanda, F. Plasser, D. R. Rehn, M. L. Vidal, Z.-Q. You, Y. Zhu, B. Alam, B. J. Albrecht, A. Aldossary, E. Alguire, J. H. Andersen, V. Athavale, D. Barton, K. Begam, A. Behn, N. Bellonzi, Y. A. Bernard, E. J. Berquist, H. G. A. Burton, A. Carreras, K. Carter-Fenk, R. Chakraborty, A. D. Chien, K. D. Closser, V. Cofer-Shabica, S. Dasgupta, M. d. Wergifosse, J. Deng, M. Diedenhofen, H. Do, S. Ehlert, P.-T. Fang, S. Fatehi, Q. Feng, T. Friedhoff, J. Gayvert, Q. Ge, G. Gidofalvi, M. Goldey, J. Gomes, C. E. González-Espinoza, S. Gulania, A. O. Gunina, M. W. D. Hanson-Heine, P. H. P. Harbach, A. Hauser, M. F. Herbst, M. H. Vera, M. Hodecker, Z. C. Holden, S. Houck, X. Huang, K. Hui, B. C. Huynh, M. Ivanov, Á. Jász, H. Ji, H. Jiang, B. Kaduk, S. Kähler, K. Khistyayev, J. Kim, G. Kis, P. Klunzinger, Z. Koczor-Benda, J. H. Koh, D. Kosenkov, L. Kouliias, T. Kowalczyk, C. M. Krauter, K. Kue, A. Kunitsa, T. Kus, I. Ladjánszki, A. Landau, K. V. Lawler, D. Lefrancois, S. Lehtola, et al., *J. Chem. Phys.* 2021, **155**, 084801.
- [2] M. Ernzerhof, G. E. Scuseria, *J. Chem. Phys.* 1999, **110**, 5029-5036.
- [3] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297-3305.
- [4] S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* 2011, **32**, 1456-1465.
- [5] P. R. Horn, Y. Mao, M. Head-Gordon, *Phys. Chem. Chem. Phys.* 2016, **18**, 23067-23079.
- [6] E. D. B. Glendening, J. K.; Reed, A. E.; Carpenter, J. E.; Bohmann, J. A.; Morales, C. M.; Weinhold F., Theoretical Chemistry Institute, University of Wisconsin, Madison, 2001.
- [7] T. Lu, F. Chen, *J. Comput. Chem.* 2012, **33**, 580-592.
- [8] K. H. Hopmann, *Organometallics* 2016, **35**, 3795-3807.
- [9] M. M. Quintal, A. Karton, M. A. Iron, A. D. Boese, J. M. L. Martin, *J. Phys. Chem. A* 2006, **110**, 709-716.
- [10] M. Steinmetz, S. Grimme, *ChemistryOpen* 2013, **2**, 115-124.
- [11] T. Weymuth, E. P. A. Couzijn, P. Chen, M. Reiher, *Journal of Chemical Theory and Computation* 2014, **10**, 3092-3103.
- [12] L. P. Wolters, F. M. Bickelhaupt, *WIREs Comput. Mol. Sci.* 2015, **5**, 324-343.
- [13] I. Fernández, F. M. Bickelhaupt, *Chem. Soc. Rev.* 2014, **43**, 4953-4967.
- [14] F. M. Bickelhaupt, *J. Comput. Chem.* 1999, **20**, 114-128.
- [15] D. H. Ess, K. N. Houk, *J. Am. Chem. Soc.* 2007, **129**, 10646-10647.
- [16] D. H. Ess, K. N. Houk, *J. Am. Chem. Soc.* 2008, **130**, 10187-10198.
- [17] F. M. Bickelhaupt, K. N. Houk, *Angew. Chem. Int. Ed.* 2017, **56**, 10070-10086.
- [18] R. Z. Khaliullin, E. A. Cobar, R. C. Lochan, A. T. Bell, M. Head-Gordon, *J. Phys. Chem. A* 2007, **111**, 8753-8765.
- [19] Y. Mao, M. Loipersberger, P. R. Horn, A. Das, O. Demerdash, D. S. Levine, S. P. Veccham, T. Head-Gordon, M. Head-Gordon, *Annu. Rev. Phys. Chem.* 2021, **72**, 641-666.
- [20] M. v. Hopffgarten, G. Frenking, *WIREs Comput. Mol. Sci.* 2012, **2**, 43-62.
- [21] N. I. Saper, A. Ohgi, D. W. Small, K. Semba, Y. Nakao, J. F. Hartwig, *Nat. Chem.* 2020, **12**, 276-283.
- [22] Y. Mao, M. Loipersberger, K. J. Kron, J. S. Derrick, C. J. Chang, S. M. Sharada, M. Head-Gordon, *Chem. Sci.* 2021, **12**, 1398-1414.
- [23] R. Z. Khaliullin, A. T. Bell, M. Head-Gordon, *Chemistry – A European Journal* 2009, **15**, 851-855.
- [24] J. Thirman, E. Engelage, S. M. Huber, M. Head-Gordon, *Phys. Chem. Chem. Phys.* 2018, **20**, 905-915.
- [25] P. R. Horn, E. J. Sundstrom, T. A. Baker, M. Head-Gordon, *J. Chem. Phys.* 2013, **138**, 134119.
- [26] E. Ben-Ari, M. Gandelman, H. Rozenberg, L. J. W. Shimon, D. Milstein, *J. Am. Chem. Soc.* 2003, **125**, 4714-4715.
- [27] L. Fan, S. Parkin, O. V. Ozerov, *J. Am. Chem. Soc.* 2005, **127**, 16772-16773.
- [28] H. Wu, M. B. Hall, *Can. J. Chem.* 2009, **87**, 1460-1469.

- [29] H. Wu, M. B. Hall, *Dalton Trans.* 2009, 5933-5942.
- [30] E. Ben-Ari, R. Cohen, M. Gandelman, L. J. W. Shimon, J. M. L. Martin, D. Milstein, *Organometallics* 2006, **25**, 3190-3210.

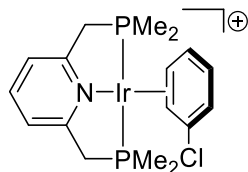
7. Atomic Coordinates of Optimized Structures



12

PhCl

| | | | |
|----|---------------|---------------|---------------|
| H | -2.1061947027 | -2.1572311959 | 0.0025503860 |
| C | -1.5656771096 | -1.2078321649 | 0.0015922233 |
| C | -0.1722221293 | -1.2150088364 | -0.0020815730 |
| H | 0.3874967102 | -2.1515391852 | -0.0039374734 |
| C | 0.5093504087 | 0.0001702929 | -0.0032438303 |
| Cl | 2.2480910851 | 0.0022044978 | -0.0079395517 |
| C | -0.1747642572 | 1.2140271194 | -0.0010278469 |
| H | 0.3828897468 | 2.1517832857 | -0.0022376803 |
| C | -1.5681473663 | 1.2039547160 | 0.0025319143 |
| H | -2.1107184647 | 2.1521801908 | 0.0043845697 |
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| H | -3.3586529638 | -0.0037927604 | 0.0065420621 |



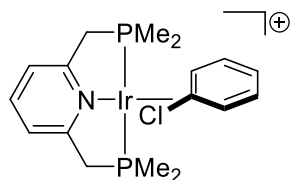
(L1)Ir-SC-1

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(L1)Ir-SC-1

| | | | |
|----|----------|----------|----------|
| Ir | -0.00971 | -0.20592 | 0.30374 |
| P | 0.69112 | 2.00314 | 0.19707 |
| P | -1.27833 | -2.09856 | 0.23783 |
| N | -1.87737 | 0.71131 | 0.10427 |
| C | -0.84082 | 2.77882 | 0.87328 |
| C | -2.03497 | 2.03051 | 0.39093 |
| C | -3.27416 | 2.65325 | 0.26191 |
| C | -4.37921 | 1.91614 | -0.14277 |
| C | -4.21262 | 0.56713 | -0.42772 |
| C | -2.95251 | -0.00985 | -0.31200 |
| C | -2.73969 | -1.44748 | -0.67247 |
| C | 1.97390 | 2.94386 | 1.08855 |
| H | 1.73265 | 4.01595 | 1.03095 |
| H | 2.01436 | 2.62697 | 2.13834 |
| H | 2.95489 | 2.77972 | 0.62851 |
| C | 0.79344 | 2.64824 | -1.50601 |
| H | -0.07571 | 2.29442 | -2.07776 |
| H | 0.82803 | 3.74758 | -1.51985 |
| H | 1.69716 | 2.24342 | -1.98393 |
| C | -1.95262 | -2.75279 | 1.80284 |
| H | -2.41367 | -1.93392 | 2.37176 |
| H | -2.69799 | -3.54013 | 1.61603 |
| H | -1.13413 | -3.17036 | 2.40639 |
| C | -0.78977 | -3.59641 | -0.67926 |

| | | | |
|----|----------|----------|----------|
| H | -1.61900 | -4.31749 | -0.72554 |
| H | 0.06039 | -4.07545 | -0.17200 |
| H | -0.48342 | -3.32714 | -1.69950 |
| H | -0.76994 | 2.67960 | 1.97029 |
| H | -0.92143 | 3.85100 | 0.64141 |
| H | -3.36525 | 3.71399 | 0.49821 |
| H | -5.36055 | 2.38616 | -0.23581 |
| H | -5.05227 | -0.04758 | -0.75562 |
| H | -3.65361 | -2.04047 | -0.51802 |
| H | -2.48196 | -1.51478 | -1.74374 |
| H | 4.30811 | 0.77382 | 1.97753 |
| C | 3.59482 | 0.22469 | 1.35893 |
| C | 3.71464 | 0.29907 | -0.05654 |
| H | 4.50767 | 0.89157 | -0.51640 |
| C | 2.83799 | -0.39594 | -0.84595 |
| Cl | 2.97710 | -0.34647 | -2.57011 |
| C | 1.80803 | -1.23176 | -0.28963 |
| H | 1.48422 | -2.06202 | -0.92116 |
| C | 1.70472 | -1.29249 | 1.13729 |
| H | 1.26539 | -2.17428 | 1.61219 |
| C | 2.61480 | -0.53155 | 1.94356 |
| H | 2.55676 | -0.61835 | 3.03047 |



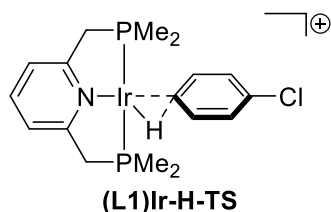
(L1)Ir-SC-2

46

(L1)Ir-SC-2

| | | | |
|----|----------|----------|----------|
| Ir | 0.05050 | 0.65815 | -0.60486 |
| P | 0.05242 | 2.90417 | -0.97108 |
| P | 0.54469 | -1.52288 | -0.11657 |
| N | 1.96245 | 0.98420 | -0.02433 |
| C | 1.86696 | 3.13060 | -1.20236 |
| C | 2.60728 | 2.14291 | -0.35452 |
| C | 3.91510 | 2.38482 | 0.04727 |
| C | 4.60793 | 1.42444 | 0.77271 |
| C | 3.95652 | 0.24100 | 1.09144 |
| C | 2.63695 | 0.04577 | 0.70021 |
| C | 1.90183 | -1.19995 | 1.08807 |
| C | -0.71343 | 3.67205 | -2.43499 |
| H | -0.42903 | 4.73046 | -2.52998 |
| H | -0.41020 | 3.12489 | -3.33796 |
| H | -1.80690 | 3.60645 | -2.33935 |
| C | -0.40775 | 4.01844 | 0.39884 |
| H | 0.11658 | 3.70602 | 1.31217 |
| H | -0.15777 | 5.06445 | 0.16627 |
| H | -1.48928 | 3.93763 | 0.57805 |
| C | 1.30265 | -2.53028 | -1.43638 |

| | | | |
|----|----------|----------|----------|
| H | 2.10167 | -1.95343 | -1.92139 |
| H | 1.71136 | -3.47111 | -1.03849 |
| H | 0.53923 | -2.75854 | -2.19348 |
| C | -0.54851 | -2.70102 | 0.74331 |
| H | 0.00588 | -3.60481 | 1.03678 |
| H | -1.37130 | -2.98672 | 0.07297 |
| H | -0.98439 | -2.22510 | 1.63149 |
| H | 2.05244 | 2.89617 | -2.26511 |
| H | 2.21698 | 4.15804 | -1.02449 |
| H | 4.38596 | 3.32735 | -0.23408 |
| H | 5.64028 | 1.59485 | 1.08288 |
| H | 4.45772 | -0.54261 | 1.66107 |
| H | 2.59048 | -2.04788 | 1.21903 |
| H | 1.39621 | -1.03284 | 2.05502 |
| H | -3.98466 | -1.82303 | -1.72083 |
| C | -3.92757 | -1.58586 | -0.65704 |
| C | -3.10379 | -0.56543 | -0.20127 |
| Cl | -2.15275 | 0.32447 | -1.39438 |
| C | -2.99577 | -0.22150 | 1.14032 |
| H | -2.32280 | 0.58288 | 1.44346 |
| C | -3.75089 | -0.94378 | 2.06257 |
| H | -3.68779 | -0.69166 | 3.12339 |
| C | -4.58514 | -1.97853 | 1.63745 |
| H | -5.17306 | -2.53884 | 2.36712 |
| C | -4.67409 | -2.29630 | 0.28305 |
| H | -5.32915 | -3.10369 | -0.05124 |

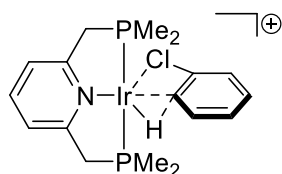


46

(L1)Ir-H-TS

| | | | |
|----|---------------|---------------|---------------|
| Ir | 0.2894193524 | -0.0688930085 | -0.3099103199 |
| P | 0.1107903806 | 2.2180999014 | -0.4161578292 |
| P | 1.1160415190 | -2.2140097556 | -0.2720662551 |
| N | 2.2604494616 | 0.3743675626 | 0.2969101364 |
| C | 1.9003729121 | 2.6630173347 | -0.4926919268 |
| C | 2.7450988270 | 1.6405982512 | 0.1986669460 |
| C | 4.0095959235 | 1.9678948853 | 0.6790321040 |
| C | 4.8100973978 | 0.9789672594 | 1.2370729532 |
| C | 4.3199973002 | -0.3188303270 | 1.3088428163 |
| C | 3.0371551203 | -0.5972609712 | 0.8461839077 |
| C | 2.4657106222 | -1.9770273460 | 0.9635445233 |
| C | -0.5888846609 | 3.1631826463 | -1.8106630727 |
| H | -0.2244340954 | 4.2009123585 | -1.7757878999 |
| H | -0.2958874201 | 2.7016333386 | -2.7631786963 |
| H | -1.6842396737 | 3.1822869702 | -1.7422169828 |
| C | -0.5445440170 | 3.0691889672 | 1.0565365163 |

| | | | |
|----|---------------|---------------|---------------|
| H | -0.0267184333 | 2.7044556086 | 1.9543872637 |
| H | -0.4294497411 | 4.1604439704 | 0.9786142999 |
| H | -1.6110085869 | 2.8177251963 | 1.1524377024 |
| C | 1.9705436899 | -2.6968366305 | -1.8099504883 |
| H | 2.6160160750 | -1.8728183133 | -2.1427701880 |
| H | 2.5729090415 | -3.6054535985 | -1.6616766305 |
| H | 1.2213815199 | -2.8811509948 | -2.5927436685 |
| C | 0.3016707358 | -3.7563779739 | 0.2592127237 |
| H | 1.0081019817 | -4.5976120635 | 0.2024346851 |
| H | -0.5535403258 | -3.9638569678 | -0.3994361526 |
| H | -0.0627037450 | -3.6636424756 | 1.2912538379 |
| H | 2.1612109952 | 2.6590749768 | -1.5658941482 |
| H | 2.1060232768 | 3.6759990479 | -0.1156498224 |
| H | 4.3638251890 | 2.9960962060 | 0.5944050021 |
| H | 5.8088153765 | 1.2170081415 | 1.6092268431 |
| H | 4.9196552257 | -1.1228963952 | 1.7375144565 |
| H | 3.2563802391 | -2.7399200285 | 0.8987667946 |
| H | 1.9892943145 | -2.0860335888 | 1.9534954455 |
| C | -4.4829480273 | -0.4935635779 | 0.5488587469 |
| C | -3.5581403991 | -1.4044156378 | 1.0593715442 |
| H | -3.8801805929 | -2.1566917412 | 1.7813834099 |
| C | -2.2346383798 | -1.3524111674 | 0.6369168590 |
| C | -1.7816347190 | -0.3592543873 | -0.2540261643 |
| C | -2.7556808481 | 0.5061384626 | -0.7898734690 |
| H | -2.4726563199 | 1.2285501222 | -1.5561407826 |
| C | -4.0873184673 | 0.4555459631 | -0.3909842453 |
| H | -4.8222519713 | 1.1424928414 | -0.8137583817 |
| H | -0.8618989218 | -0.5419575943 | -1.3421813275 |
| Cl | -6.1303549055 | -0.5616768090 | 1.0649924278 |
| H | -1.5362048485 | -2.0797376635 | 1.0478190968 |



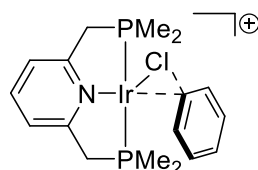
(L1)Ir-H-TS'

46

(L1)Ir-H-TS'

| | | | |
|----|---------------|---------------|---------------|
| Ir | 0.0731194393 | 0.1583378132 | 0.1132008161 |
| P | -0.2250197147 | -2.1156774593 | -0.1858212144 |
| P | 0.9362681706 | 2.2544564152 | 0.3396088371 |
| N | 2.0896693600 | -0.3643786107 | -0.1004417659 |
| C | 1.4443686240 | -2.6840235817 | 0.3556021072 |
| C | 2.4818649643 | -1.6616346311 | 0.0094203026 |
| C | 3.8142032788 | -2.0266490423 | -0.1626396237 |
| C | 4.7678059584 | -1.0495120621 | -0.4173276183 |
| C | 4.3618777942 | 0.2759715545 | -0.5125811025 |
| C | 3.0153265411 | 0.5962124592 | -0.3685816638 |
| C | 2.5419931916 | 2.0091053868 | -0.5370043459 |
| C | -1.3771070245 | -3.2363565458 | 0.6601236720 |

| | | | |
|----|---------------|---------------|---------------|
| H | -1.1420103519 | -4.2785796521 | 0.3976460514 |
| H | -1.3123317775 | -3.0940630997 | 1.7456141337 |
| H | -2.4029978224 | -3.0052360039 | 0.3435162745 |
| C | -0.3506322141 | -2.6091026629 | -1.9381953563 |
| H | 0.4427759260 | -2.1189899822 | -2.5192533743 |
| H | -0.2766129300 | -3.7002414455 | -2.0572825184 |
| H | -1.3199388996 | -2.2643205075 | -2.3264222788 |
| C | 1.3891798252 | 2.7938763300 | 2.0208114690 |
| H | 1.9592378588 | 1.9963636069 | 2.5165718202 |
| H | 1.9856223293 | 3.7179294275 | 1.9949199301 |
| H | 0.4721362716 | 2.9692983823 | 2.6006414672 |
| C | 0.2021613982 | 3.7367864837 | -0.4200945496 |
| H | 0.8594357221 | 4.6101198221 | -0.2971828709 |
| H | -0.7627159279 | 3.9431875684 | 0.0648125072 |
| H | 0.0205234695 | 3.5625193488 | -1.4891204873 |
| H | 1.3845203258 | -2.7708088733 | 1.4547928124 |
| H | 1.7157878259 | -3.6757956317 | -0.0359524075 |
| H | 4.0954732947 | -3.0770804999 | -0.0770367925 |
| H | 5.8190130288 | -1.3183917431 | -0.5407847898 |
| H | 5.0813676858 | 1.0702352954 | -0.7158591006 |
| H | 3.3186567592 | 2.7274260200 | -0.2341967567 |
| H | 2.3332570650 | 2.1897129403 | -1.6059714485 |
| H | -5.5560528085 | 0.6834516405 | -1.8327777570 |
| C | -4.5621196913 | 0.6428628387 | -1.3826731851 |
| C | -3.4669078709 | 1.2149183215 | -2.0309581349 |
| H | -3.5959804963 | 1.7062179244 | -2.9977872226 |
| C | -2.2058529208 | 1.1702748945 | -1.4455568645 |
| H | -1.3587522727 | 1.6211788633 | -1.9666683661 |
| C | -1.9831644055 | 0.5089934285 | -0.2210733687 |
| C | -3.1202833183 | -0.0034149388 | 0.4306253533 |
| Cl | -2.9670909450 | -0.6638935100 | 2.0359931185 |
| C | -4.3920391490 | 0.0444442524 | -0.1392907995 |
| H | -5.2402329773 | -0.3710189854 | 0.4070468344 |
| H | -1.1833130582 | 0.7791010236 | 0.9115164795 |



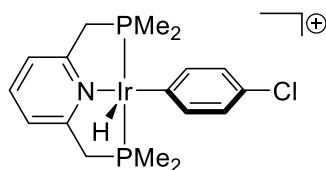
(L1)Ir-Cl-TS

46

(L1)Ir-Cl-TS

| | | | |
|----|---------------|---------------|---------------|
| Ir | -0.1286887046 | -0.0351098356 | -0.4871899343 |
| P | 0.4174162963 | -2.2723668774 | -0.6262554990 |
| P | 0.1414731467 | 2.2459504355 | -0.4337544435 |
| N | 1.6776455094 | -0.0043136968 | 0.4591629858 |
| C | 1.3094541914 | -2.3575694562 | 0.9874049176 |
| C | 2.1364294332 | -1.1174369046 | 1.1001149509 |
| C | 3.3403132991 | -1.1027407281 | 1.7969812945 |
| C | 4.0989829148 | 0.0597993409 | 1.8444585832 |

| | | | |
|----|---------------|---------------|---------------|
| C | 3.6506258525 | 1.1754900451 | 1.1462365154 |
| C | 2.4537425876 | 1.1176605406 | 0.4423833057 |
| C | 1.9844510435 | 2.2545013363 | -0.4070767394 |
| C | -0.6220437308 | -3.7712493329 | -0.6813965113 |
| H | 0.0090557339 | -4.6578135904 | -0.8384178895 |
| H | -1.1774654424 | -3.8973848995 | 0.2568054452 |
| H | -1.3381177543 | -3.6921357945 | -1.5119147211 |
| C | 1.6907772833 | -2.6140517397 | -1.8883627232 |
| H | 2.4512074756 | -1.8218976890 | -1.8637644949 |
| H | 2.1661686303 | -3.5926475167 | -1.7242971843 |
| H | 1.2179224503 | -2.6016819547 | -2.8806587182 |
| C | -0.2605681458 | 3.2610779617 | 1.0319715021 |
| H | 0.0602502038 | 2.7297203073 | 1.9389124741 |
| H | 0.2515424274 | 4.2330818967 | 0.9733194890 |
| H | -1.3417982910 | 3.4305789051 | 1.1013760912 |
| C | -0.3323947026 | 3.2906206230 | -1.8458551063 |
| H | 0.0928183204 | 4.3009822575 | -1.7558391098 |
| H | -1.4285419544 | 3.3669849976 | -1.8831416939 |
| H | 0.0102771629 | 2.8213009063 | -2.7777933131 |
| H | 0.5160595188 | -2.3592267059 | 1.7560340383 |
| H | 1.9240915150 | -3.2596024696 | 1.1241293092 |
| H | 3.6698095196 | -2.0107811992 | 2.3036554206 |
| H | 5.0381812894 | 0.0906434450 | 2.4001737330 |
| H | 4.2350276125 | 2.0962170172 | 1.1225930791 |
| H | 2.4162495590 | 3.2118083143 | -0.0812190518 |
| H | 2.3079670526 | 2.0745085703 | -1.4470291679 |
| H | -3.2393200458 | -2.1701765341 | 2.7606438009 |
| C | -3.0856390848 | -1.2386044144 | 2.2108751099 |
| C | -2.5380064139 | -1.2907808242 | 0.9317817025 |
| H | -2.3170437982 | -2.2434296807 | 0.4583839598 |
| C | -2.2969611392 | -0.0909939839 | 0.2435610998 |
| Cl | -2.1907986361 | -0.1648363791 | -1.6612679531 |
| C | -2.7980040620 | 1.1212209299 | 0.7480152048 |
| H | -2.7661905052 | 2.0190099522 | 0.1301981786 |
| C | -3.3475510237 | 1.1500584718 | 2.0231846940 |
| H | -3.7094852037 | 2.0990234647 | 2.4260976208 |
| C | -3.4704395577 | -0.0220536706 | 2.7731292295 |
| H | -3.9127698740 | 0.0075722919 | 3.7703799828 |



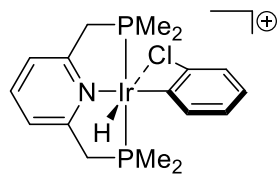
(L1)Ir(H)(Ar)

46

(L1)Ir(H)(Ar)

| | | | |
|----|--------------|---------------|---------------|
| H | 0.4625790293 | -0.0545889842 | 1.5470520180 |
| Ir | 0.3494001501 | 0.0082719182 | 0.0183443522 |
| P | 0.4453661570 | 2.2961190223 | 0.1778721883 |
| P | 0.8350329766 | -2.2366069985 | -0.0567472495 |

| | | | |
|----|---------------|---------------|---------------|
| N | 2.4912948590 | 0.2123526093 | -0.1363719395 |
| C | 2.1051675934 | 2.5854708309 | -0.5976589605 |
| C | 3.0402837758 | 1.4263881845 | -0.3779597955 |
| C | 4.4207182322 | 1.5797570399 | -0.4686715233 |
| C | 5.2397922012 | 0.4637387558 | -0.3369633789 |
| C | 4.6634087021 | -0.7764051693 | -0.0891715956 |
| C | 3.2794641981 | -0.8739433487 | 0.0298955834 |
| C | 2.6241174686 | -2.1728226627 | 0.4170931017 |
| C | -0.7163204181 | 3.3476406691 | -0.7402685136 |
| H | -0.4299468243 | 4.4082904535 | -0.6943370495 |
| H | -0.7649105565 | 3.0192320668 | -1.7875487921 |
| H | -1.7142963057 | 3.2147215056 | -0.2979346879 |
| C | 0.5390300967 | 3.0293526497 | 1.8404203548 |
| H | 1.3247927029 | 2.5251140026 | 2.4194198190 |
| H | 0.7526854167 | 4.1067891411 | 1.7867079956 |
| H | -0.4223238583 | 2.8784117352 | 2.3514799408 |
| C | 0.7954955127 | -3.1023271653 | -1.6620486029 |
| H | 1.3428514274 | -2.5209890683 | -2.4172281529 |
| H | 1.2470406548 | -4.1018137630 | -1.5758477449 |
| H | -0.2483288665 | -3.2109348711 | -1.9891540812 |
| C | 0.0514298098 | -3.3888690726 | 1.1057416965 |
| H | 0.5102378319 | -4.3870862900 | 1.0608714248 |
| H | -1.0137335498 | -3.4617729025 | 0.8429104826 |
| H | 0.1244716631 | -2.9874265129 | 2.1253365418 |
| H | 1.9106941279 | 2.6807698322 | -1.6810644868 |
| H | 2.5632672101 | 3.5335046551 | -0.2782939622 |
| H | 4.8431750604 | 2.5670653273 | -0.6597464345 |
| H | 6.3239329457 | 0.5608939933 | -0.4222972821 |
| H | 5.2795487892 | -1.6683937790 | 0.0333018544 |
| H | 3.1909021195 | -3.0357966435 | 0.0364424800 |
| H | 2.6384381969 | -2.2483199858 | 1.5190485085 |
| H | -4.5119913076 | 0.8367250645 | 1.7183223527 |
| C | -3.8877439511 | 0.3747920144 | 0.9511382879 |
| C | -2.4991626914 | 0.4386644382 | 1.0262321691 |
| H | -2.0564783911 | 0.9624296329 | 1.8786729436 |
| C | -1.6665309112 | -0.1563862685 | 0.0587157259 |
| C | -2.3154438842 | -0.8336479006 | -0.9920062309 |
| H | -1.7281376740 | -1.3326672016 | -1.7713795027 |
| C | -3.7048639091 | -0.8884166286 | -1.1014140912 |
| H | -4.1825568157 | -1.4071526703 | -1.9345806357 |
| C | -4.4873415910 | -0.2839578576 | -0.1221647063 |
| Cl | -6.2155527959 | -0.3564515283 | -0.2341368956 |

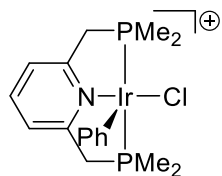


(L1)Ir(H)(Ar)⁺

46

(L1)Ir(H)(Ar)⁺

| | | | |
|----|---------------|---------------|---------------|
| H | -0.2677536641 | -0.0525582217 | 1.8489713440 |
| Ir | -0.0286199203 | -0.0372176884 | 0.3150948296 |
| P | -0.2026042854 | -2.3294646291 | 0.2860529895 |
| P | -0.4719234338 | 2.2084594725 | 0.4032737097 |
| N | -2.1210859401 | -0.1588080935 | -0.0872650357 |
| C | -1.6941054438 | -2.4611520091 | -0.8011251014 |
| C | -2.6342232538 | -1.3118892961 | -0.5697268347 |
| C | -3.9892900066 | -1.4158123564 | -0.8778417139 |
| C | -4.8124808358 | -0.3082953357 | -0.7150939089 |
| C | -4.2674548284 | 0.8750543601 | -0.2289512078 |
| C | -2.9138516595 | 0.9216985299 | 0.0961778458 |
| C | -2.2955870857 | 2.1424797492 | 0.7128613800 |
| C | 1.0560508955 | -3.3882300497 | -0.4819630855 |
| H | 0.7039308210 | -4.4248615265 | -0.5829850807 |
| H | 1.3188801852 | -2.9835131000 | -1.4687356623 |
| H | 1.9562465573 | -3.3675060734 | 0.1484778026 |
| C | -0.6578720830 | -3.1671368065 | 1.8348302881 |
| H | -1.5233131800 | -2.6583224863 | 2.2812164111 |
| H | -0.9023392752 | -4.2244430006 | 1.6564480490 |
| H | 0.1839139493 | -3.1017881322 | 2.5382213278 |
| C | -0.2672327192 | 3.1958986820 | -1.1116734195 |
| H | -0.7862939239 | 2.7020696117 | -1.9446369336 |
| H | -0.6640884961 | 4.2130896735 | -0.9793043969 |
| H | 0.8027334718 | 3.2509449218 | -1.3578287150 |
| C | 0.2113656031 | 3.2366436005 | 1.7335265462 |
| H | -0.2275878177 | 4.2447970036 | 1.7334186557 |
| H | 1.2980993751 | 3.3115534715 | 1.5857253650 |
| H | 0.0284088243 | 2.7487252666 | 2.7002720034 |
| H | -1.3074806147 | -2.4005198652 | -1.8342082244 |
| H | -2.2153645660 | -3.4261954568 | -0.7111442157 |
| H | -4.3864422265 | -2.3584662141 | -1.2576908349 |
| H | -5.8743788264 | -0.3676728538 | -0.9636816337 |
| H | -4.8898940279 | 1.7590292669 | -0.0831413284 |
| H | -2.8176568105 | 3.0580968438 | 0.3980751877 |
| H | -2.4068318881 | 2.0692381958 | 1.8093380928 |
| H | 5.0815468791 | 0.2392230531 | 1.8350927195 |
| C | 4.3295831951 | 0.1847277581 | 1.0442805895 |
| C | 2.9743124227 | 0.1394179239 | 1.3862342194 |
| H | 2.6810891797 | 0.1564415986 | 2.4391840853 |
| C | 1.9917972181 | 0.0671773677 | 0.3908889427 |
| C | 2.4731526394 | 0.0483385608 | -0.9167802783 |
| Cl | 1.1230104578 | -0.0437913193 | -2.0953983070 |
| C | 3.7955006639 | 0.0901664163 | -1.3151888894 |
| H | 4.0823320168 | 0.0710650205 | -2.3680540108 |
| C | 4.7413517818 | 0.1603519010 | -0.2895159086 |
| H | 5.8034337815 | 0.1963405827 | -0.5394104734 |



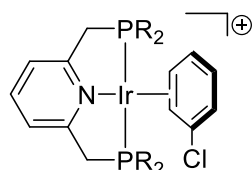
(L1)Ir(CI)(Ph)

46

(L1)Ir(CI)(Ph)

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| Ir | 0.3768427002 | 0.2013618634 | 0.3009567185 |
| P | -0.8654413731 | 2.0902487239 | 0.7776118296 |
| P | 1.2796285537 | -1.9022716169 | 0.0057228422 |
| N | -1.2301054460 | -0.8216764583 | 1.0582469298 |
| C | -2.0541705808 | 1.3212271524 | 1.9648579505 |
| C | -2.2000911963 | -0.1552914627 | 1.7401358779 |
| C | -3.2993470772 | -0.8376182570 | 2.2554267559 |
| C | -3.3944629494 | -2.2151590617 | 2.1058765670 |
| C | -2.3834265367 | -2.8849995647 | 1.4293290616 |
| C | -1.3163547046 | -2.1696196000 | 0.8950077090 |
| C | -0.2895995660 | -2.8617215944 | 0.0485737863 |
| C | -0.0919451802 | 3.4606765235 | 1.6797422095 |
| H | -0.8412761717 | 4.1887433676 | 2.0228185400 |
| H | 0.4702834327 | 3.0665518245 | 2.5371341548 |
| H | 0.6226453491 | 3.9541699006 | 1.0062327375 |
| C | -1.8559411819 | 2.8644869607 | -0.5319488058 |
| H | -2.4594352248 | 2.1040798836 | -1.0444044545 |
| H | -2.5050256664 | 3.6459009603 | -0.1114529307 |
| H | -1.1728695553 | 3.3097805120 | -1.2690798576 |
| C | 2.3120674798 | -2.5402891640 | 1.3588187478 |
| H | 1.7794400112 | -2.4309403938 | 2.3141043583 |
| H | 2.5614899080 | -3.5995951977 | 1.1992506366 |
| H | 3.2372426923 | -1.9480913647 | 1.4047525123 |
| C | 2.1254323943 | -2.3510635200 | -1.5301501238 |
| H | 2.3275128499 | -3.4309538649 | -1.5717530419 |
| H | 3.0745500554 | -1.7978233916 | -1.5709910581 |
| H | 1.5060145627 | -2.0474451200 | -2.3849750061 |
| H | -4.0737346689 | -0.2785582540 | 2.7824730284 |
| H | -4.2496778813 | -2.7613826071 | 2.5094011214 |
| H | -2.4265690950 | -3.9653313518 | 1.2833678526 |
| H | -0.1594142747 | -3.9096151581 | 0.3546792801 |
| H | -0.6565472520 | -2.8665048412 | -0.9936815721 |
| H | 0.5109412149 | 0.8539359224 | -4.7163450899 |
| C | -0.1308906482 | 0.4933491659 | -3.9086392304 |
| C | -1.4079911176 | 0.0110942099 | -4.1883885177 |
| H | -1.7776817418 | -0.0141305928 | -5.2154165178 |
| C | -2.2070552206 | -0.4315457339 | -3.1395275774 |
| H | -3.2142814972 | -0.8066300494 | -3.3379785779 |
| C | -1.7399518697 | -0.3980993650 | -1.8219853831 |
| H | -2.4146247714 | -0.7395356691 | -1.0359656058 |
| C | -0.4524234246 | 0.0766010693 | -1.5360980064 |
| C | 0.3464969727 | 0.5279581962 | -2.5991296407 |
| H | 1.3467280007 | 0.9144926020 | -2.4032156565 |

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|----|---------------|--------------|--------------|
| H | -3.0383960831 | 1.8130182086 | 1.9646077808 |
| H | -1.6262979969 | 1.4780979358 | 2.9707686072 |
| Cl | 2.3921821180 | 1.3218310932 | 0.0405506085 |



(tBuL1)Ir-SC-1

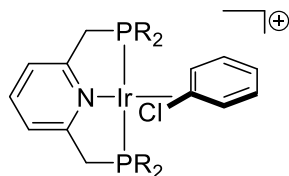
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82

(tBuL1)Ir-SC-1

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| Ir | -0.1186240283 | -0.1977797654 | -0.0202883607 |
| P | 2.0907655705 | 0.6612189782 | 0.1710248995 |
| P | -2.4512081468 | -0.2672196056 | -0.0781983369 |
| N | -0.5327487563 | 1.8117433703 | -0.4950840708 |
| C | 1.5702885657 | 2.4034802428 | 0.5380678102 |
| C | 0.3480037675 | 2.7953357264 | -0.1992528063 |
| C | 0.0976544813 | 4.1281650128 | -0.5202684596 |
| C | -1.0949791789 | 4.4737900627 | -1.1382359388 |
| C | -2.0139340984 | 3.4671891640 | -1.4103505868 |
| C | -1.7119488829 | 2.1503433052 | -1.0809911009 |
| C | -2.6737100454 | 1.0510880567 | -1.3521030770 |
| C | 3.2115278110 | 0.4041963976 | 1.6911661717 |
| C | 3.1098104889 | 0.8687310899 | -1.4174607735 |
| C | -3.1753152946 | 0.4504605716 | 1.5323067917 |
| C | -3.5606316537 | -1.6483857428 | -0.7743088001 |
| H | 1.3278577283 | 2.4028961519 | 1.6136316834 |
| H | 2.3753504355 | 3.1341815657 | 0.3906247532 |
| H | 0.8418688735 | 4.8837200126 | -0.2655908921 |
| H | -1.3115782367 | 5.5125795891 | -1.3956151344 |
| H | -2.9703936290 | 3.6897263793 | -1.8849363155 |
| H | -3.7006862252 | 1.4278439218 | -1.4484447664 |
| H | -2.3979822082 | 0.5701828611 | -2.3029735925 |
| H | 3.0040659197 | -3.8396517829 | 1.3498495253 |
| C | 2.1802056062 | -3.3578639671 | 0.8189177533 |
| C | 2.2038919035 | -3.3310322293 | -0.6031293465 |
| H | 3.0404991398 | -3.7662401910 | -1.1520351292 |
| C | 1.1365910945 | -2.8087635427 | -1.2774027084 |
| Cl | 1.0600357694 | -2.8747276297 | -3.0068921251 |
| C | -0.0100488132 | -2.2780997552 | -0.6008521544 |
| H | -0.9387627266 | -2.3882692903 | -1.1545110072 |
| C | 0.0003547359 | -2.2668414978 | 0.8306112697 |
| H | -0.9422743066 | -2.2979893960 | 1.3817134637 |
| C | 1.1235834308 | -2.8360762665 | 1.5148222282 |
| H | 1.0842902921 | -2.9386725092 | 2.6013085768 |
| C | -4.4070099232 | 1.3262958193 | 1.2995805709 |
| H | -4.7501838853 | 1.7182026815 | 2.2704533637 |
| H | -4.1753232786 | 2.1979000742 | 0.6700099984 |
| H | -5.2483984031 | 0.7869521552 | 0.8503184249 |

| | | | |
|---|---------------|---------------|---------------|
| C | -2.0933190479 | 1.3165679277 | 2.1928940835 |
| H | -1.8820036414 | 2.2283472072 | 1.6188745752 |
| H | -2.4534622687 | 1.6285007906 | 3.1859977500 |
| H | -1.1486070896 | 0.7628683870 | 2.3154454607 |
| C | -3.5029069337 | -0.6935963567 | 2.4945202255 |
| H | -4.3435898663 | -1.3114877165 | 2.1549171188 |
| H | -2.6334318460 | -1.3463495783 | 2.6665837496 |
| H | -3.7858153587 | -0.2674286455 | 3.4697497728 |
| C | -5.0442360214 | -1.2793959788 | -0.6934949952 |
| H | -5.4212025373 | -1.2651321250 | 0.3369105256 |
| H | -5.2657054843 | -0.3092782470 | -1.1611238450 |
| H | -5.6231239567 | -2.0415980867 | -1.2387284792 |
| C | -3.2120112956 | -1.8378801474 | -2.2602012904 |
| H | -3.6661713311 | -2.7783065137 | -2.6085260648 |
| H | -3.6267172428 | -1.0337056793 | -2.8837369025 |
| H | -2.1339946742 | -1.9006421554 | -2.4678809281 |
| C | -3.3391772021 | -2.9717492177 | -0.0301738032 |
| H | -4.0466013870 | -3.7164279663 | -0.4275720312 |
| H | -2.3312211292 | -3.3794127563 | -0.1715564343 |
| H | -3.5260134029 | -2.8910401955 | 1.0471024802 |
| C | 2.2808857333 | 0.0525042272 | 2.8551548527 |
| H | 1.5255890363 | 0.8330644945 | 3.0376608454 |
| H | 1.7498233078 | -0.8883939656 | 2.6848321965 |
| H | 2.8773562560 | -0.0454620318 | 3.7762024821 |
| C | 3.9967106442 | 1.6626349854 | 2.0854886302 |
| H | 4.6406252958 | 2.0448963337 | 1.2853206804 |
| H | 3.3516471369 | 2.4789920213 | 2.4363152086 |
| H | 4.6525536635 | 1.3972745508 | 2.9297469534 |
| C | 4.2118393328 | -0.7253836281 | 1.4528469368 |
| H | 3.7276849901 | -1.6352575373 | 1.0824960336 |
| H | 4.9945533274 | -0.4293074534 | 0.7415930039 |
| H | 4.7096464513 | -0.9727607555 | 2.4036835059 |
| C | 3.6235111617 | -0.4826490909 | -1.9152227233 |
| H | 2.8036602618 | -1.1322538666 | -2.2383610849 |
| H | 4.2599974681 | -0.3078133350 | -2.7972445050 |
| H | 4.2291301249 | -1.0180157316 | -1.1741518290 |
| C | 2.1452736692 | 1.4231298450 | -2.4727318296 |
| H | 1.2413814648 | 0.8003613826 | -2.5572962143 |
| H | 1.8408755190 | 2.4592123223 | -2.2649123694 |
| H | 2.6516881135 | 1.4234111951 | -3.4507880442 |
| C | 4.2932833106 | 1.8231965102 | -1.2611856682 |
| H | 4.7293811915 | 2.0035790380 | -2.2565851042 |
| H | 4.0112131851 | 2.8047184166 | -0.8542295975 |
| H | 5.0899872555 | 1.4007729048 | -0.6347109139 |



(tBuL1)Ir-SC-2

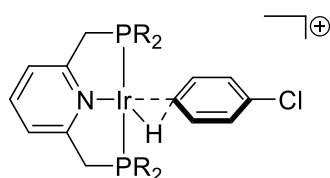
R = tBu

82

(tBuL1)Ir-SC-2

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| Ir | -0.0232229702 | -0.1736654247 | 0.0828599307 |
| P | -2.2133171826 | 0.5723871495 | 0.1108324103 |
| P | 1.9242243583 | -1.4308966303 | 0.0923006597 |
| N | -0.8301209809 | -1.8864798620 | -0.6453623275 |
| C | -3.0179746993 | -1.0894403000 | 0.1138718240 |
| C | -2.1730676809 | -2.1049336700 | -0.5782671270 |
| C | -2.7492652765 | -3.2663726730 | -1.0842833799 |
| C | -1.9493704794 | -4.2549143649 | -1.6404073572 |
| C | -0.5770711867 | -4.0479000991 | -1.6709616059 |
| C | -0.0403912184 | -2.8623688347 | -1.1785218855 |
| C | 1.4283845064 | -2.6150968504 | -1.2375253395 |
| C | -2.8924472135 | 1.3457351672 | 1.6967397046 |
| C | -2.8663523064 | 1.4080253171 | -1.4486894851 |
| C | 2.0669300239 | -2.4823563032 | 1.6648904133 |
| C | 3.6085004842 | -0.7993359917 | -0.4979651503 |
| H | -3.0808524646 | -1.3767964203 | 1.1764953088 |
| H | -4.0448898942 | -1.0927277697 | -0.2781579785 |
| H | -3.8309296659 | -3.3901775618 | -1.0163576143 |
| H | -2.3866884335 | -5.1744420658 | -2.0341103361 |
| H | 0.0964379328 | -4.7981428657 | -2.0872619335 |
| H | 1.9899184137 | -3.5592432901 | -1.2475753228 |
| H | 1.6501243578 | -2.0916120765 | -2.1796594214 |
| H | 1.9288501356 | 4.3816910962 | 1.5112046709 |
| C | 1.9294562025 | 4.1747426545 | 0.4395136674 |
| C | 1.4424665620 | 2.9716698228 | -0.0555408273 |
| Cl | 0.8359708708 | 1.7839521839 | 1.1016849952 |
| C | 1.4253030527 | 2.6611195335 | -1.4076469329 |
| H | 1.0185089636 | 1.6931888935 | -1.7163010448 |
| C | 1.9235549553 | 3.6033710363 | -2.3057036931 |
| H | 1.9203184730 | 3.3817980624 | -3.3752470131 |
| C | 2.4201340721 | 4.8212281949 | -1.8423620768 |
| H | 2.8086790037 | 5.5562959919 | -2.5499826672 |
| C | 2.4213257886 | 5.1041560004 | -0.4761341181 |
| H | 2.8099544847 | 6.0581014143 | -0.1134423987 |
| C | 3.4499905072 | -0.3810395192 | -1.9653263825 |
| H | 4.3092404272 | 0.2446434512 | -2.2523633854 |
| H | 3.4388241774 | -1.2437723766 | -2.6465481809 |
| H | 2.5392779946 | 0.2113655199 | -2.1339107253 |
| C | 4.7149071650 | -1.8493480817 | -0.4059257563 |
| H | 5.6195174794 | -1.4546430359 | -0.8955640562 |
| H | 4.9860035055 | -2.0806287826 | 0.6327167326 |
| H | 4.4508849330 | -2.7867749047 | -0.9178960777 |

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| C | 2.7581834281 | -1.6461061114 | 2.7436891334 |
| H | 3.8268323155 | -1.4975895718 | 2.5381612975 |
| H | 2.2826420273 | -0.6591133177 | 2.8571596443 |
| H | 2.6806942224 | -2.1667910379 | 3.7111846613 |
| C | 2.7878576381 | -3.8151437285 | 1.4690733181 |
| H | 3.8351235806 | -3.7048545549 | 1.1674060298 |
| H | 2.7787558918 | -4.3650518041 | 2.4237900565 |
| H | 2.2783742047 | -4.4529767361 | 0.7320971656 |
| C | 0.6335754827 | -2.7763566737 | 2.1259570288 |
| H | 0.6716198447 | -3.3016709701 | 3.0934891044 |
| H | 0.0535935733 | -1.8475611643 | 2.2403630675 |
| H | 0.0956760056 | -3.4261125933 | 1.4199732108 |
| C | -2.1261269853 | 0.6933638117 | 2.8538055333 |
| H | -1.0504500165 | 0.9076069191 | 2.8130343991 |
| H | -2.5178826146 | 1.0812995928 | 3.8075032933 |
| H | -2.2439528585 | -0.4005352794 | 2.8725322376 |
| C | -2.6328572405 | 2.8540631759 | 1.7070864696 |
| H | -1.5835300674 | 3.0996874095 | 1.4889828297 |
| H | -3.2717195783 | 3.3870053474 | 0.9899222086 |
| H | -2.8671567209 | 3.2504637361 | 2.7076655021 |
| C | -4.3876448499 | 1.0813925263 | 1.8948300248 |
| H | -4.7042632879 | 1.5429250267 | 2.8437148177 |
| H | -5.0067711043 | 1.5125419427 | 1.0999831401 |
| H | -4.6202158963 | 0.0096178045 | 1.9693852117 |
| C | -2.1325291771 | 2.7342892086 | -1.6562660412 |
| H | -1.0440783880 | 2.5978709505 | -1.6570518985 |
| H | -2.4197337314 | 3.1563263731 | -2.6323853567 |
| H | -2.3793131149 | 3.4792759990 | -0.8901282329 |
| C | -4.3746790913 | 1.6440400359 | -1.4474952440 |
| H | -4.6724030884 | 2.4187225661 | -0.7282139280 |
| H | -4.6826213487 | 1.9952212750 | -2.4453203869 |
| H | -4.949907167 | 0.7307704016 | -1.2347186946 |
| C | -2.4947158541 | 0.4628297716 | -2.5978153039 |
| H | -1.4179467622 | 0.2322052955 | -2.5938517830 |
| H | -3.0504145791 | -0.4858228512 | -2.5604683000 |
| H | -2.7412075426 | 0.9477251982 | -3.5554503739 |
| C | 3.9999332642 | 0.4389332891 | 0.3142029722 |
| H | 4.9884932642 | 0.7871528617 | -0.0243061232 |
| H | 3.2926013958 | 1.2617777946 | 0.1605468030 |
| H | 4.0703029355 | 0.2428090428 | 1.3909786783 |



(tBuL1)Ir-H-TS

R = tBu

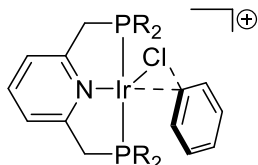
82

(tBuL1)Ir-H-TS

| | | | |
|----|--------------|--------------|---------------|
| Ir | 0.2497410792 | 0.0631522163 | -0.0584150591 |
|----|--------------|--------------|---------------|

| | | | |
|----|---------------|---------------|---------------|
| P | -1.1997413183 | 1.8998517227 | -0.1869240138 |
| P | 2.1696584590 | -1.2388239975 | -0.0305876890 |
| N | 1.5893245715 | 1.4987351120 | 0.6880417378 |
| C | 0.0921751520 | 3.2240413707 | -0.1632795301 |
| C | 1.3086391397 | 2.8210973000 | 0.5966944744 |
| C | 2.1602489269 | 3.7827983923 | 1.1356702845 |
| C | 3.3411964757 | 3.3880310714 | 1.7490465478 |
| C | 3.6437573702 | 2.0330416439 | 1.8035798891 |
| C | 2.7515286131 | 1.1060655401 | 1.2731196108 |
| C | 3.0440099528 | -0.3570472541 | 1.3398306194 |
| C | -2.1136719726 | 2.3106348902 | -1.7931232769 |
| C | -2.2380520883 | 2.2450807219 | 1.3492285929 |
| C | 3.2264381494 | -0.9239661686 | -1.5761329274 |
| C | 2.1953387263 | -3.0563065557 | 0.4854636858 |
| H | -0.2871373285 | 4.1971632613 | 0.1779856451 |
| H | 1.8948102421 | 4.8373428662 | 1.0509064480 |
| H | 4.0239927704 | 4.1282774946 | 2.1713886198 |
| H | 4.5666716794 | 1.6805130300 | 2.2656276143 |
| H | 4.1260765395 | -0.5429385187 | 1.3819491696 |
| H | 2.6093160246 | -0.7567070073 | 2.2687385074 |
| C | -3.6859523026 | -2.8739308570 | 0.1269739012 |
| C | -2.7620310004 | -2.7294173522 | 1.1638211797 |
| H | -2.9499959039 | -3.2041321979 | 2.1283774533 |
| C | -1.6094108948 | -1.9812849354 | 0.9591247820 |
| C | -1.3650993963 | -1.3155729788 | -0.2595974048 |
| C | -2.2978820590 | -1.5151477281 | -1.2899642410 |
| H | -2.1244219873 | -1.0744160412 | -2.2733394653 |
| C | -3.4501194463 | -2.2789205318 | -1.1072722254 |
| H | -4.1605183349 | -2.4156518600 | -1.9242067526 |
| H | -0.2432718163 | -1.1112253829 | -1.0490762485 |
| Cl | -5.1180426071 | -3.8099878207 | 0.3772104823 |
| H | -0.9104623490 | -1.8727781956 | 1.7889688098 |
| C | 2.9671607552 | 0.5182672806 | -2.0287839404 |
| H | 3.4863940021 | 0.6855104590 | -2.9856147721 |
| H | 1.8911736095 | 0.7065794115 | -2.1645867368 |
| H | 3.3564100115 | 1.2552875584 | -1.3120003614 |
| C | 2.7597514784 | -1.8649129662 | -2.6887437001 |
| H | 3.0012469768 | -2.9155328693 | -2.4815456556 |
| H | 1.6760006565 | -1.7814564677 | -2.8636625647 |
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| C | 4.7274124434 | -1.0829340581 | -1.3297345212 |
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| H | 5.2626823655 | -0.8632858954 | -2.2671406173 |
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| C | 3.5698813185 | -3.7127515746 | 0.3550910815 |
| H | 3.5170399001 | -4.7250070922 | 0.7861601192 |
| H | 3.8873725586 | -3.8238065881 | -0.6900286969 |
| H | 4.3506531349 | -3.1661922976 | 0.9047153902 |
| C | 1.7684796326 | -3.1214296971 | 1.9568697055 |
| H | 1.5098482591 | -4.1620245557 | 2.2059773983 |
| H | 2.5761328004 | -2.8176354416 | 2.6380357827 |
| H | 0.8845587035 | -2.5037182822 | 2.1653111950 |

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| C | 1.1691861799 | -3.8185785891 | -0.3610428704 |
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| H | 0.1508634871 | -3.4376350506 | -0.2129579801 |
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| H | 0.3923466343 | 3.3526806778 | -1.2165933286 |
| C | -1.2641618929 | 1.7244737295 | -2.9258250267 |
| H | -1.1781310345 | 0.6327612952 | -2.8595637138 |
| H | -1.7251313714 | 1.9786367010 | -3.8933924952 |
| H | -0.2408669033 | 2.1304783227 | -2.9317308097 |
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| H | -3.4973321207 | 0.6219716513 | -1.5203166070 |
| H | -4.1948532610 | 2.2089225505 | -1.1229462663 |
| H | -3.9304602143 | 1.7603039586 | -2.8143627232 |
| C | -2.2502094192 | 3.8205720533 | -2.0201435519 |
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| C | -3.2697226677 | 1.1293107714 | 1.5370920944 |
| H | -2.7985852074 | 0.1398273717 | 1.5891301190 |
| H | -3.8038633458 | 1.2986274385 | 2.4854133040 |
| H | -4.0202836629 | 1.1056934662 | 0.7381416847 |
| C | -2.9379527053 | 3.6021451966 | 1.3242401885 |
| H | -3.7284184713 | 3.6464940461 | 0.5634929923 |
| H | -3.4177072353 | 3.7745535626 | 2.3007367795 |
| H | -2.2433607279 | 4.4381956407 | 1.1540470555 |
| C | -1.2531032286 | 2.1974973408 | 2.5238701415 |
| H | -0.6863039434 | 1.2531869797 | 2.5357573535 |
| H | -0.5366140393 | 3.0321463305 | 2.5089964461 |
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(tBuL1)Ir-Cl-TS

R = tBu

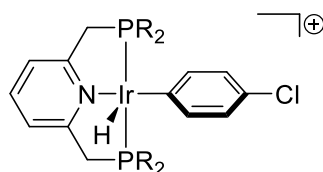
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(tBuL1)Ir-Cl-TS

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| P | 2.4070004688 | -0.1261481114 | 0.0405402287 |
| P | -2.1809494373 | -0.5409172639 | 0.3539411925 |
| N | 0.1703944592 | -1.5505431716 | -0.9969336440 |
| C | 2.3975419707 | -0.8457325892 | -1.6662986126 |
| C | 1.2573516695 | -1.7934998948 | -1.7782606717 |
| C | 1.3244771848 | -2.9097761245 | -2.6072798896 |
| C | 0.2795740883 | -3.8239811775 | -2.6247714122 |
| C | -0.7807539237 | -3.6260385930 | -1.7485951105 |
| C | -0.7978168990 | -2.5058821178 | -0.9253693918 |
| C | -1.8131924730 | -2.3375632925 | 0.1441843783 |
| C | 3.8015651925 | 1.1772501637 | -0.0729409264 |

| | | | |
|----|---------------|---------------|---------------|
| C | 2.9304340170 | -1.5191339493 | 1.2354438244 |
| C | -3.4017164275 | -0.2389611666 | -1.0940431167 |
| C | -3.0377622727 | -0.5124030539 | 2.0386002095 |
| H | 2.2240917683 | 0.0156763055 | -2.3295417035 |
| H | 3.3402869109 | -1.3212432003 | -1.9710905006 |
| H | 2.2079379612 | -3.0506282217 | -3.2312686403 |
| H | 0.3087796410 | -4.6955694134 | -3.2814855608 |
| H | -1.5909685089 | -4.3521961671 | -1.6706218595 |
| H | -2.6914946087 | -2.9711844089 | -0.0188369255 |
| H | -1.3439396348 | -2.6537824089 | 1.0888297974 |
| H | 0.8950377322 | 4.2108263222 | -2.6117688760 |
| C | 0.1407882657 | 3.8092229961 | -1.9306930281 |
| C | 0.5465201686 | 2.9743254061 | -0.8926840757 |
| H | 1.5956517657 | 2.7674501490 | -0.7288596100 |
| C | -0.4122928047 | 2.4079683331 | -0.0475390986 |
| Cl | 0.1070053100 | 1.9164594370 | 1.7372374908 |
| C | -1.7445912470 | 2.8384353338 | -0.1230120068 |
| H | -2.4571653132 | 2.5109746291 | 0.6297444621 |
| C | -2.1307481687 | 3.6907702512 | -1.1497170863 |
| H | -3.1755222974 | 4.0041076858 | -1.2151451795 |
| C | -1.1997015905 | 4.1609754426 | -2.0779708580 |
| H | -1.5104153067 | 4.8331444439 | -2.8795967800 |
| C | -4.4410676461 | 0.8403013210 | -0.7841681795 |
| H | -3.9947420679 | 1.7936239622 | -0.4874355839 |
| H | -5.0263853903 | 1.0295023929 | -1.6978319170 |
| H | -5.1499897679 | 0.5261602973 | -0.0064301644 |
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| H | -4.7274217119 | -1.9506300502 | -0.6424845170 |
| H | -4.8891489992 | -1.2577013173 | -2.2628225317 |
| H | -3.5017897770 | -2.2847528679 | -1.9006799145 |
| C | -2.5501037200 | 0.1907722521 | -2.2948505017 |
| H | -1.9910602446 | 1.1139159372 | -2.1008000435 |
| H | -1.8299309254 | -0.5875645845 | -2.5842652918 |
| H | -3.2131624255 | 0.3633272108 | -3.1577711126 |
| C | -3.3933633495 | 0.9210048169 | 2.4431886226 |
| H | -2.4956812377 | 1.5486173616 | 2.5273428731 |
| H | -4.1029329335 | 1.3985971436 | 1.7563629590 |
| H | -3.8692366989 | 0.8989027595 | 3.4361180556 |
| C | -4.2893389625 | -1.3904236054 | 2.0553223632 |
| H | -4.7062092436 | -1.4013851187 | 3.0748616580 |
| H | -5.0747019438 | -1.0151921633 | 1.3866264125 |
| H | -4.0727549425 | -2.4338918949 | 1.7843552626 |
| C | -2.0256952960 | -1.0464546884 | 3.0602649632 |
| H | -1.0648587434 | -0.5157823741 | 2.9945806878 |
| H | -2.4322475649 | -0.8978346419 | 4.0727104864 |
| H | -1.8366462839 | -2.1234910884 | 2.9480540428 |
| C | 1.7454606656 | -2.4664665864 | 1.4647575288 |
| H | 2.0196870717 | -3.1698942434 | 2.2662993914 |
| H | 0.8432684906 | -1.9158268846 | 1.7721948271 |
| H | 1.5083281144 | -3.0636987696 | 0.5737579294 |
| C | 3.2492764859 | -0.8678195949 | 2.5855206235 |
| H | 4.1465371616 | -0.2377132371 | 2.5639930712 |

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| H | 2.4047218552 | -0.2565059409 | 2.9409272072 |
| H | 3.4236465238 | -1.6575023683 | 3.3330225969 |
| C | 4.0933893510 | -2.3703975174 | 0.7227916194 |
| H | 5.0313713126 | -1.8198947074 | 0.6106217769 |
| H | 4.2765302446 | -3.1842472874 | 1.4423699136 |
| H | 3.8513625775 | -2.8456821614 | -0.2398341243 |
| C | 3.5727280615 | 2.2408684174 | 1.0080988371 |
| H | 4.3753060956 | 2.9924220475 | 0.9464166442 |
| H | 2.6147216542 | 2.7629878235 | 0.9042315891 |
| H | 3.5986752143 | 1.8130359008 | 2.0188749644 |
| C | 5.2086746480 | 0.5988206171 | 0.1018879934 |
| H | 5.9307564602 | 1.4140232696 | -0.0638633482 |
| H | 5.3964893202 | 0.2050192930 | 1.1077084158 |
| H | 5.4335670891 | -0.1845984633 | -0.6350940577 |
| C | 3.7859322408 | 1.8111022211 | -1.4738310999 |
| H | 4.2588444501 | 1.1500954718 | -2.2137747901 |
| H | 2.7894390628 | 2.0667165562 | -1.8526397877 |
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(tBuL1)Ir(H)(Ar)

R = tBu

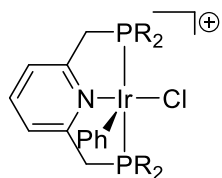
82

(tBuL1)Ir(H)(Ar)

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| Ir | 0.1838266846 | 0.1269010174 | 0.0991830293 |
| P | -0.8291088183 | 2.2099678575 | -0.1420686238 |
| P | 1.7027139357 | -1.6056354828 | 0.3267233574 |
| N | 1.9762531951 | 1.3154825121 | -0.0110263940 |
| C | 0.5956228622 | 3.1246358031 | -0.9053055960 |
| C | 1.9264175449 | 2.5834412585 | -0.4741202365 |
| C | 3.0852652121 | 3.3499423333 | -0.5888111427 |
| C | 4.3099105355 | 2.7919494514 | -0.2433017530 |
| C | 4.3476317181 | 1.4852146626 | 0.2316077705 |
| C | 3.1592755944 | 0.7697896859 | 0.3558973447 |
| C | 3.1331354444 | -0.6037672454 | 0.9526787134 |
| C | -2.1908849177 | 2.3873604666 | -1.4263544218 |
| C | -1.1802894318 | 3.1276844840 | 1.4663380065 |
| C | 2.2462242572 | -2.1996709364 | -1.3859179353 |
| C | 1.5023135953 | -2.9813061566 | 1.5918637292 |
| H | 0.4983659156 | 2.9707628387 | -1.9931098825 |
| H | 0.5418408427 | 4.2111765215 | -0.7434831629 |
| H | 3.0200348367 | 4.3728169194 | -0.9628102063 |
| H | 5.2297033079 | 3.3728148239 | -0.3391430695 |
| H | 5.2903825547 | 1.0211325362 | 0.5249911129 |
| H | 4.1047041604 | -1.1037251615 | 0.8472106376 |
| H | 2.9472335232 | -0.4922157263 | 2.0330970871 |

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| C | -3.4583304134 | -2.0128253346 | 1.2267718045 |
| C | -2.3309440854 | -1.1924445299 | 1.2488817779 |
| H | -2.1059743557 | -0.6729816440 | 2.1825040867 |
| C | -1.4914845123 | -1.0293221885 | 0.1314469283 |
| C | -1.8571006146 | -1.7559526945 | -1.0190224715 |
| H | -1.2456841338 | -1.6944373728 | -1.9258951634 |
| C | -2.9814755034 | -2.5786483603 | -1.0692721613 |
| H | -3.2349720507 | -3.1256971647 | -1.9792346618 |
| C | -3.7825419580 | -2.7043981171 | 0.0623234627 |
| Cl | -5.1822061429 | -3.7288731896 | 0.0217977959 |
| C | 3.7456054857 | -2.4820705173 | -1.4750487286 |
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| C | 1.4583584859 | -3.4434773435 | -1.7983934101 |
| H | 1.7628234709 | -4.3291200430 | -1.2259263085 |
| H | 0.3735236625 | -3.3117537504 | -1.6822351603 |
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| C | 1.8943703542 | -1.0499730713 | -2.3424170510 |
| H | 2.0847511220 | -1.3631630290 | -3.3813409306 |
| H | 0.8224391222 | -0.7793108105 | -2.2882472342 |
| H | 2.4923932478 | -0.1476184996 | -2.1554161642 |
| C | 1.2438105826 | -2.3011620232 | 2.9415583789 |
| H | 0.3801393489 | -1.6222234227 | 2.8915469727 |
| H | 1.0124402232 | -3.0783431129 | 3.6858121930 |
| H | 2.1126132199 | -1.7448107918 | 3.3212140389 |
| C | 0.2725192389 | -3.8338341252 | 1.2591053352 |
| H | 0.1131869045 | -4.5445671574 | 2.0850015002 |
| H | -0.6349390863 | -3.2235014002 | 1.1611457597 |
| H | 0.3946385798 | -4.4228790269 | 0.3441038948 |
| C | 2.7558875795 | -3.8522792230 | 1.6714957241 |
| H | 2.6298677948 | -4.5942355370 | 2.4755813598 |
| H | 2.9303823145 | -4.4102404693 | 0.7412076486 |
| H | 3.6608678292 | -3.2712414570 | 1.9037604409 |
| C | -1.7908452336 | 1.4552991648 | -2.5762739573 |
| H | -1.7503915612 | 0.4091684483 | -2.2476875070 |
| H | -2.5487073095 | 1.5223767694 | -3.3722522955 |
| H | -0.8253700088 | 1.7271223390 | -3.0312176377 |
| C | -2.3413584181 | 3.8074719622 | -1.9746219259 |
| H | -3.1007019437 | 3.7946557364 | -2.7724266371 |
| H | -2.6763466761 | 4.5274048757 | -1.2201212956 |
| H | -1.4117207038 | 4.1856600844 | -2.4245218291 |
| C | -3.5093415476 | 1.8939318831 | -0.8242454011 |
| H | -3.4126232178 | 0.8855628071 | -0.3948748393 |
| H | -3.8905010734 | 2.5729879173 | -0.0489635082 |
| H | -4.2703755950 | 1.8475581395 | -1.6187799495 |
| C | -2.0623677135 | 2.2479764231 | 2.3548102436 |
| H | -1.5393164304 | 1.3253169779 | 2.6397331812 |
| H | -2.3045484855 | 2.7973122787 | 3.2779633551 |
| H | -3.0067215660 | 1.9638103019 | 1.8735764035 |
| C | -1.8452624162 | 4.4843806296 | 1.2438279256 |

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| H | -2.8703908527 | 4.3870201748 | 0.8628117567 |
| H | -1.9064078129 | 5.0120193598 | 2.2086613363 |
| H | -1.2762409772 | 5.1286926466 | 0.5571685209 |
| C | 0.1661363661 | 3.3387906518 | 2.1682563341 |
| H | 0.7176558242 | 2.3963245008 | 2.2982416076 |
| H | 0.8132939689 | 4.0496735472 | 1.6348211246 |
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(tBuL1)Ir(Cl)(Ph)

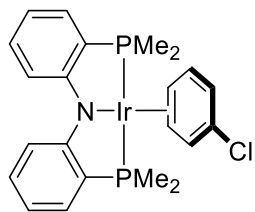
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82

(tBuL1)Ir(Cl)(Ph)

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| P | -2.3379334338 | 0.0231434369 | 0.1001562744 |
| N | -0.0568080169 | 0.6157377180 | -1.6712311872 |
| C | 2.2629906302 | 1.4050984174 | -1.4116199375 |
| C | 1.0503275283 | 1.1487357727 | -2.2500179182 |
| C | 1.0374597047 | 1.5550713377 | -3.5829264411 |
| C | -0.1353459727 | 1.4780859461 | -4.3202624928 |
| C | -1.2793733561 | 0.9931213021 | -3.6987843521 |
| C | -1.2176036026 | 0.5528239847 | -2.3806310965 |
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| C | 2.9436536823 | 1.7024333193 | 1.4097964411 |
| C | -2.8705045460 | 1.7725047011 | 0.5716438220 |
| C | -3.5309650009 | -1.3006260033 | 0.7201650591 |
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| H | -0.1617259167 | 1.8036849435 | -5.3621214971 |
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| H | -3.3476030371 | 0.3214998450 | -2.1706916200 |
| H | -2.3835696536 | -1.1472093028 | -1.9556776326 |
| H | 0.0535324077 | -5.0334552831 | 1.2030972024 |
| C | 0.0227836600 | -4.2900612307 | 0.4025984110 |
| C | -0.0688332534 | -4.6956330930 | -0.9271307310 |
| H | -0.1125440917 | -5.7559271299 | -1.1838145624 |
| C | -0.0926382815 | -3.7243473946 | -1.9231320172 |
| H | -0.1465287833 | -4.0163856459 | -2.9750018064 |
| C | -0.0393635234 | -2.3673298460 | -1.5963642657 |
| H | -0.0302265186 | -1.6506292793 | -2.4168610786 |
| C | 0.0285095692 | -1.9468614674 | -0.2593091289 |
| C | 0.0713208352 | -2.9366022287 | 0.7372079341 |
| H | 0.1407154673 | -2.6494414852 | 1.7851860021 |
| H | 3.1817145844 | 1.3104454424 | -2.0072289257 |
| H | 2.2129301113 | 2.4623199736 | -1.1010229890 |
| Cl | -0.0057225111 | -0.2757937559 | 2.6287963463 |
| C | -1.6810976017 | 2.6780063860 | 0.2278678279 |

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| H | -1.8943714485 | 3.7020489991 | 0.5730184988 |
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| C | -3.0965057512 | 1.8300787716 | 2.0846443753 |
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| H | -3.2284063409 | 2.8811494294 | 2.3860649773 |
| C | -4.9865601704 | -0.8377382196 | 0.6342406173 |
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| H | -5.6333093689 | -1.6790254758 | 0.9285190310 |
| H | -5.2101590541 | -0.0052717205 | 1.3132253401 |
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| H | -3.9613814742 | -3.3643638919 | 0.3336742694 |
| C | 1.7684678031 | 2.6437493660 | 1.6967960569 |
| H | 1.3968449671 | 3.1474353491 | 0.7900851391 |
| H | 0.9398236176 | 2.1153876041 | 2.1880020258 |
| H | 2.1088983908 | 3.4359392963 | 2.3816264775 |
| C | 4.1125534025 | 2.5460838550 | 0.8905705823 |
| H | 3.8676295412 | 3.1003284314 | -0.0273269013 |
| H | 4.3561727904 | 3.2979857863 | 1.6574830657 |
| H | 5.0208701795 | 1.9634052389 | 0.7079993065 |
| C | 3.3378799646 | 0.9951335452 | 2.7087722766 |
| H | 2.5260020145 | 0.3548363240 | 3.0815797238 |
| H | 4.2492354804 | 0.3932138154 | 2.5957699260 |
| H | 3.5457281537 | 1.7569627253 | 3.4765233967 |
| C | 5.0239465282 | -0.4224185881 | -0.1727717515 |
| H | 5.6830355427 | -1.2529929024 | -0.4705206392 |
| H | 5.1697726808 | 0.3852061416 | -0.9057386669 |
| H | 5.3673923595 | -0.0737367794 | 0.8091218171 |
| C | 3.5869631412 | -0.9421542401 | -0.1443974811 |
| C | 3.4317606639 | -1.9989014106 | 0.9526986408 |
| H | 4.1698882741 | -2.7978824265 | 0.7799593256 |
| H | 3.6082464234 | -1.5942280574 | 1.9571190816 |
| H | 2.4349239781 | -2.4551703014 | 0.9362750209 |
| C | 3.2762393749 | -1.5698285243 | -1.5061444232 |
| H | 3.4409271900 | -0.8710872096 | -2.3396578174 |
| H | 3.9588247003 | -2.4200813457 | -1.6593911525 |
| H | 2.2536591242 | -1.9580792621 | -1.5639049186 |



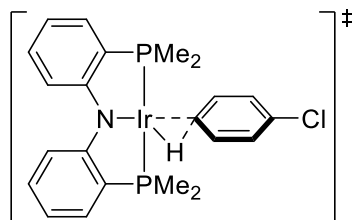
(L3)Ir-SC-1

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(L3)Ir-SC-1

| | | | |
|----|----------|----------|----------|
| Ir | -0.17498 | -0.54454 | 0.32688 |
| P | -0.92237 | 1.62121 | -0.01401 |
| P | 1.09623 | -2.37079 | 0.83300 |
| N | 1.62525 | 0.41062 | 0.56945 |
| C | -1.23968 | 2.25366 | -1.70317 |
| H | -1.29764 | 3.35214 | -1.70278 |
| H | -0.41778 | 1.93135 | -2.35614 |
| H | -2.18108 | 1.82979 | -2.07734 |
| C | -2.28533 | 2.35387 | 0.96080 |
| H | -2.14417 | 2.09119 | 2.01756 |
| H | -2.30053 | 3.44722 | 0.85091 |
| H | -3.24132 | 1.94021 | 0.62002 |
| C | 0.99149 | -3.90041 | -0.16638 |
| H | 1.15654 | -3.64928 | -1.22273 |
| H | 1.73580 | -4.64428 | 0.15230 |
| H | -0.01155 | -4.33860 | -0.05511 |
| C | 1.03671 | -3.00687 | 2.54875 |
| H | 1.82351 | -3.75662 | 2.71881 |
| H | 0.05303 | -3.45690 | 2.74719 |
| H | 1.17932 | -2.16178 | 3.23494 |
| Cl | -4.79498 | 0.46717 | -2.19172 |
| C | -3.69820 | -0.34155 | -1.11138 |
| C | -3.99746 | -0.35956 | 0.28702 |
| H | -4.89833 | 0.12330 | 0.66912 |
| C | -3.15189 | -1.00395 | 1.14026 |
| H | -3.38160 | -1.04747 | 2.20591 |
| C | -1.96272 | -1.68855 | 0.69856 |
| H | -1.69738 | -2.55737 | 1.30918 |
| C | -1.67561 | -1.66415 | -0.72025 |
| H | -1.14683 | -2.50611 | -1.17803 |
| C | -2.58817 | -0.96999 | -1.59721 |
| H | -2.39873 | -0.99546 | -2.67347 |
| C | 0.52755 | 2.55911 | 0.55712 |
| C | 1.66149 | 1.77176 | 0.86222 |
| C | 2.80238 | -0.31731 | 0.41084 |
| C | 2.76328 | -1.72395 | 0.57973 |
| C | 2.73275 | 2.41764 | 1.51694 |
| C | 2.70528 | 3.78518 | 1.75893 |
| C | 1.61506 | 4.56743 | 1.37298 |
| C | 0.52228 | 3.93468 | 0.78859 |
| H | 3.58673 | 1.83375 | 1.85991 |
| H | 3.55238 | 4.24731 | 2.27283 |

| | | | |
|---|----------|----------|----------|
| H | 1.60381 | 5.64330 | 1.55721 |
| H | -0.36170 | 4.52298 | 0.52562 |
| C | 3.90926 | -2.50814 | 0.45277 |
| C | 5.13010 | -1.93307 | 0.11403 |
| C | 5.16955 | -0.55809 | -0.12803 |
| C | 4.03833 | 0.23643 | 0.01123 |
| H | 3.84222 | -3.58974 | 0.60168 |
| H | 6.02648 | -2.54679 | 0.00801 |
| H | 6.10441 | -0.09015 | -0.44796 |
| H | 4.10359 | 1.29947 | -0.21935 |



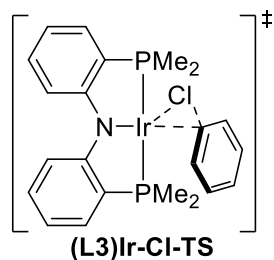
(L3)Ir-H-TS

52

(L3)Ir-H-TS

| | | | |
|----|----------|----------|----------|
| Ir | 0.06844 | -0.36483 | -0.43318 |
| P | -1.27898 | -2.19064 | -0.61119 |
| P | 0.91108 | 1.74865 | -0.16771 |
| N | -1.67840 | 0.54239 | 0.12046 |
| C | -1.85917 | -2.71921 | -2.26854 |
| H | -2.67035 | -3.45780 | -2.18189 |
| H | -2.22585 | -1.83530 | -2.80661 |
| H | -1.02484 | -3.15797 | -2.83516 |
| C | -0.83082 | -3.79435 | 0.15990 |
| H | -0.61697 | -3.63084 | 1.22505 |
| H | -1.63973 | -4.53373 | 0.06601 |
| H | 0.06919 | -4.19495 | -0.33038 |
| C | 1.84640 | 2.58533 | -1.50399 |
| H | 1.31999 | 2.43661 | -2.45608 |
| H | 1.93646 | 3.66257 | -1.30238 |
| H | 2.85332 | 2.15322 | -1.57302 |
| C | 1.91549 | 2.14924 | 1.31145 |
| H | 2.07319 | 3.23446 | 1.40101 |
| H | 2.88804 | 1.64121 | 1.24153 |
| H | 1.38733 | 1.78158 | 2.20085 |
| C | -4.79584 | -1.96462 | 1.52047 |
| C | -3.77477 | -2.45407 | 0.71384 |
| C | -2.74089 | -1.62205 | 0.28242 |
| C | -2.71351 | -0.24070 | 0.60687 |
| C | -3.72614 | 0.21859 | 1.48262 |
| C | -4.73787 | -0.62530 | 1.91816 |
| H | -5.60031 | -2.61762 | 1.86377 |
| H | -3.76863 | -3.51063 | 0.42974 |
| H | -3.69754 | 1.24464 | 1.84792 |
| H | -5.49402 | -0.22901 | 2.60134 |
| C | -3.02191 | 2.61544 | -0.07636 |

| | | | |
|----|----------|----------|----------|
| C | -1.79372 | 1.92085 | 0.03425 |
| C | -0.61528 | 2.70693 | -0.02458 |
| C | -0.67262 | 4.10105 | -0.06731 |
| C | -1.89225 | 4.76682 | -0.10240 |
| C | -3.06167 | 4.00100 | -0.13623 |
| H | -3.95375 | 2.05484 | -0.14422 |
| H | 0.25770 | 4.67672 | -0.09157 |
| H | -1.93408 | 5.85694 | -0.13969 |
| H | -4.03248 | 4.49572 | -0.22716 |
| C | 4.38189 | -0.66866 | 0.67059 |
| C | 3.34622 | -1.39629 | 1.24141 |
| H | 3.41110 | -1.71417 | 2.28266 |
| C | 2.23613 | -1.72759 | 0.45121 |
| C | 2.16030 | -1.26042 | -0.86842 |
| C | 3.22335 | -0.53895 | -1.42533 |
| H | 3.14840 | -0.18151 | -2.45454 |
| C | 4.35175 | -0.25578 | -0.66899 |
| H | 5.19679 | 0.29327 | -1.08652 |
| H | 1.28489 | -1.52488 | -1.52881 |
| H | 1.47070 | -2.39058 | 0.85392 |
| Cl | 5.76519 | -0.25952 | 1.63725 |

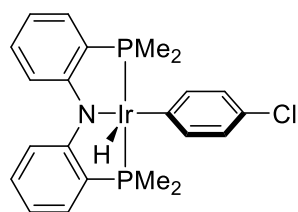


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(L3)Ir-Cl-TS

| | | | |
|----|----------|----------|----------|
| Ir | -0.41598 | -0.33295 | -0.57159 |
| P | 0.72760 | -2.27898 | -0.27047 |
| P | -0.65328 | 1.81902 | -1.30954 |
| N | 1.24876 | 0.49613 | 0.25511 |
| C | 0.41357 | -3.62272 | 0.94604 |
| H | 1.27881 | -4.29968 | 1.00510 |
| H | 0.23301 | -3.17880 | 1.93388 |
| H | -0.46748 | -4.20738 | 0.64366 |
| C | 0.98222 | -3.25256 | -1.80383 |
| H | 1.33645 | -2.57489 | -2.59103 |
| H | 1.71468 | -4.05972 | -1.65268 |
| H | 0.02255 | -3.68884 | -2.11788 |
| C | -2.17014 | 2.81906 | -1.55754 |
| H | -2.66867 | 2.98792 | -0.59415 |
| H | -1.93023 | 3.79242 | -2.01028 |
| H | -2.85366 | 2.27928 | -2.22896 |
| C | 0.24294 | 2.12962 | -2.87979 |
| H | 0.35267 | 3.20880 | -3.06626 |
| H | -0.29995 | 1.65987 | -3.71262 |
| H | 1.23361 | 1.66342 | -2.80064 |

| | | | |
|----|----------|----------|----------|
| C | 1.17706 | 1.82462 | 0.66226 |
| C | 1.87015 | 2.35951 | 1.76600 |
| C | 1.72250 | 3.69687 | 2.11791 |
| C | 0.88500 | 4.54961 | 1.39647 |
| C | 0.16545 | 4.02895 | 0.32231 |
| C | 0.29573 | 2.68866 | -0.03343 |
| H | 2.50093 | 1.70827 | 2.37153 |
| H | 2.26202 | 4.07596 | 2.98993 |
| H | 0.77518 | 5.59731 | 1.68319 |
| H | -0.51776 | 4.67491 | -0.23601 |
| C | 3.50358 | -2.43414 | 0.28010 |
| C | 4.74847 | -1.86722 | 0.52402 |
| C | 4.82905 | -0.47500 | 0.63694 |
| C | 3.70101 | 0.32691 | 0.55168 |
| C | 2.41543 | -0.23520 | 0.35528 |
| C | 2.35818 | -1.64191 | 0.17808 |
| H | 3.42114 | -3.51749 | 0.14751 |
| H | 5.64273 | -2.48878 | 0.59735 |
| H | 5.80219 | 0.00210 | 0.78202 |
| H | 3.81469 | 1.40896 | 0.61090 |
| H | -2.73433 | -2.48314 | 3.40961 |
| C | -2.85738 | -1.67846 | 2.68064 |
| C | -2.54607 | -1.92248 | 1.34791 |
| H | -2.20149 | -2.90088 | 1.01884 |
| C | -2.66332 | -0.87482 | 0.42466 |
| Cl | -2.52696 | -1.26436 | -1.32660 |
| C | -3.23601 | 0.34962 | 0.79491 |
| H | -3.42442 | 1.10997 | 0.04021 |
| C | -3.53697 | 0.56978 | 2.13483 |
| H | -3.94632 | 1.53760 | 2.43387 |
| C | -3.33364 | -0.43028 | 3.08675 |
| H | -3.57417 | -0.24806 | 4.13579 |



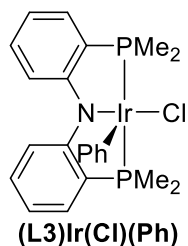
(L3)Ir(H)(Ar)

52

(L3)Ir(H)(Ar)

| | | | |
|----|---------------|---------------|---------------|
| Ir | 0.1145333101 | 0.0662317379 | -0.2674152466 |
| P | -0.0687904062 | -2.1794118568 | -0.6430000610 |
| P | -0.2711618216 | 2.2998596805 | 0.0270356165 |
| N | -1.9313891511 | -0.0903565178 | 0.1700282087 |
| C | -0.0654568271 | -2.7901706322 | -2.3631928378 |
| H | -0.3501546887 | -3.8518553344 | -2.4013489770 |
| H | -0.7804316043 | -2.1982247450 | -2.9493848445 |
| H | 0.9403196914 | -2.6640581756 | -2.7889365469 |
| C | 1.0776565123 | -3.3091103716 | 0.2169718424 |

| | | | |
|----|---------------|---------------|---------------|
| H | 1.0311041602 | -3.1097771218 | 1.2958424890 |
| H | 0.8377103456 | -4.3653014258 | 0.0274366879 |
| H | 2.0972247043 | -3.0900780583 | -0.1324834968 |
| C | 0.2380303693 | 3.4449711707 | -1.2967728344 |
| H | -0.1753162758 | 3.0889381500 | -2.2493925530 |
| H | -0.1082136344 | 4.4707497681 | -1.1051785300 |
| H | 1.3357243329 | 3.4324365606 | -1.3573532252 |
| C | 0.3081083950 | 3.1292047287 | 1.5500380194 |
| H | -0.0823795035 | 4.1557266319 | 1.6132023969 |
| H | 1.4073889298 | 3.1500892009 | 1.5519300853 |
| H | -0.0392429530 | 2.5585241805 | 2.4218520589 |
| C | 4.9379767204 | 0.0957153837 | 0.4078100947 |
| C | 4.0422415767 | 0.2718380966 | 1.4592257328 |
| H | 4.4150675649 | 0.3945032061 | 2.4781995221 |
| C | 2.6751877542 | 0.2897317174 | 1.1878512450 |
| C | 2.1475137573 | 0.1295098307 | -0.1107570901 |
| C | 3.0985087677 | -0.0434086980 | -1.1364326087 |
| H | 2.7607504962 | -0.1730814070 | -2.1687795204 |
| C | 4.4723725790 | -0.0624842779 | -0.8936837699 |
| H | 5.1834375944 | -0.1992697552 | -1.7111665428 |
| H | 0.5197715804 | 0.2913335070 | -1.7325850628 |
| H | 1.9898236544 | 0.4293525474 | 2.0329467830 |
| Cl | 6.6534724730 | 0.0769919274 | 0.7256715146 |
| C | -3.4001971088 | -3.9941743452 | 0.9577893869 |
| C | -2.2056477592 | -3.7903067418 | 0.2746741704 |
| C | -1.7188449995 | -2.5033093258 | 0.0429568967 |
| C | -2.4480385701 | -1.3513284378 | 0.4536599468 |
| C | -3.6192962922 | -1.5877003079 | 1.2079516358 |
| C | -4.0807411989 | -2.8766716494 | 1.4445738684 |
| H | -3.7743484549 | -5.0030098076 | 1.1408395915 |
| H | -1.6251892601 | -4.6525276308 | -0.0673860253 |
| H | -4.1584185426 | -0.7457644855 | 1.6407524758 |
| H | -4.9903522028 | -3.0096073642 | 2.0363311745 |
| C | -4.1231868491 | 1.0552638340 | -0.0858312473 |
| C | -2.7202926495 | 1.0525082455 | 0.0859286321 |
| C | -2.0849215827 | 2.3271868144 | 0.0754501379 |
| C | -2.8240554938 | 3.5087581402 | 0.0101402620 |
| C | -4.2109779404 | 3.4838529526 | -0.0932645038 |
| C | -4.8422163867 | 2.2413434516 | -0.1691179953 |
| H | -4.6553561616 | 0.1108456346 | -0.1893212095 |
| H | -2.2999675804 | 4.4693614445 | 0.0189551837 |
| H | -4.7849790414 | 4.4105831420 | -0.1482152146 |
| H | -5.9253992376 | 2.1898655495 | -0.3087431584 |

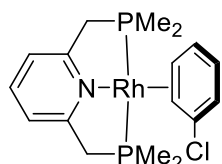


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(L3)Ir(Cl)(Ph)

| | | | |
|----|----------|----------|----------|
| Ir | 0.18288 | -0.62487 | -0.70465 |
| P | -2.10884 | -0.83115 | -0.75762 |
| P | 2.37687 | 0.03936 | -0.50482 |
| N | -0.24181 | 1.31081 | -0.16201 |
| C | -2.57299 | 0.69811 | 0.08588 |
| C | -1.50392 | 1.60137 | 0.33809 |
| C | 0.77288 | 2.25131 | -0.25217 |
| C | 2.12859 | 1.82160 | -0.31893 |
| C | -2.91899 | -0.84244 | -2.39273 |
| H | -4.01331 | -0.79609 | -2.29243 |
| H | -2.57188 | 0.02421 | -2.97128 |
| H | -2.62875 | -1.76275 | -2.91980 |
| C | -2.88993 | -2.20765 | 0.13867 |
| H | -2.52649 | -2.20521 | 1.17455 |
| H | -3.98592 | -2.12531 | 0.12310 |
| H | -2.58265 | -3.14680 | -0.34302 |
| C | 3.43796 | -0.18998 | -1.96958 |
| H | 2.95070 | 0.26932 | -2.83980 |
| H | 4.43120 | 0.25900 | -1.82574 |
| H | 3.53482 | -1.26955 | -2.15305 |
| C | 3.40016 | -0.55896 | 0.87733 |
| H | 4.35533 | -0.01555 | 0.91277 |
| H | 3.58741 | -1.63289 | 0.73608 |
| H | 2.85207 | -0.41834 | 1.81768 |
| H | 0.35269 | -4.14095 | 2.97091 |
| C | 0.29740 | -3.06345 | 2.79264 |
| C | 0.26568 | -2.17633 | 3.86774 |
| H | 0.29169 | -2.54721 | 4.89501 |
| C | 0.20344 | -0.80948 | 3.60964 |
| H | 0.17954 | -0.09458 | 4.43667 |
| C | 0.17063 | -0.33019 | 2.29846 |
| H | 0.12970 | 0.74558 | 2.13458 |
| C | 0.19607 | -1.21598 | 1.20998 |
| C | 0.26434 | -2.59434 | 1.47961 |
| H | 0.29865 | -3.30276 | 0.65106 |
| Cl | 0.63574 | -2.62117 | -1.89881 |
| C | 1.60471 | 4.54264 | -0.43330 |
| H | 1.38188 | 5.60898 | -0.52500 |
| C | 2.93390 | 4.11009 | -0.40488 |
| H | 3.75763 | 4.82472 | -0.44872 |
| C | 3.17816 | 2.74322 | -0.37075 |
| H | 4.20874 | 2.37721 | -0.40779 |
| C | -3.08270 | 2.92461 | 1.65291 |
| C | -4.13944 | 2.07105 | 1.32823 |
| H | -5.14836 | 2.26070 | 1.69863 |
| C | -3.86246 | 0.94715 | 0.55897 |
| H | -4.66131 | 0.23355 | 0.33665 |
| H | -3.25835 | 3.78246 | 2.30737 |
| C | -1.79722 | 2.69954 | 1.17946 |
| H | -0.99652 | 3.36767 | 1.49430 |

| | | | |
|---|----------|---------|----------|
| C | 0.54994 | 3.64455 | -0.36754 |
| H | -0.47020 | 4.02014 | -0.43666 |



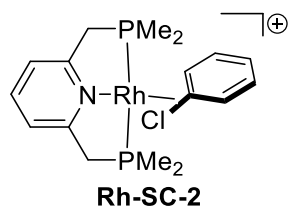
Rh-SC-1

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Rh-SC-1

| | | | |
|----|---------------|---------------|---------------|
| Rh | -0.0018574783 | 0.2997037345 | 0.2837914084 |
| P | -0.7014496717 | -1.9066835060 | 0.2229041213 |
| P | 1.2825079981 | 2.1758115899 | 0.1615992433 |
| N | 1.8571694760 | -0.6154709942 | -0.0782568808 |
| C | 0.8856740553 | -2.6692834179 | 0.7862468653 |
| C | 2.0420387205 | -1.9283150604 | 0.2004224832 |
| C | 3.2628534554 | -2.5554957542 | -0.0389174847 |
| C | 4.3218620658 | -1.8187796661 | -0.5537170998 |
| C | 4.1279203078 | -0.4708028376 | -0.8320730200 |
| C | 2.8824894056 | 0.1053594009 | -0.5987346304 |
| C | 2.6119071021 | 1.5370271816 | -0.9406276716 |
| C | -1.9123632275 | -2.8574957018 | 1.2029336137 |
| H | -1.6741963472 | -3.9294986189 | 1.1310958563 |
| H | -1.8835267624 | -2.5406299540 | 2.2534241306 |
| H | -2.9239293445 | -2.6966967836 | 0.8128166277 |
| C | -0.9226777823 | -2.5615119396 | -1.4665104528 |
| H | -0.0950540077 | -2.2141897276 | -2.1004908560 |
| H | -0.9587851133 | -3.6610096277 | -1.4722448108 |
| H | -1.8570463534 | -2.1604342071 | -1.8849316340 |
| C | 2.1493251881 | 2.6965544415 | 1.6808559242 |
| H | 2.6181228273 | 1.8197193041 | 2.1486915275 |
| H | 2.9170085053 | 3.4543299162 | 1.4639808344 |
| H | 1.4221505812 | 3.1149528908 | 2.3912920396 |
| C | 0.7594795762 | 3.7437620607 | -0.6082526235 |
| H | 1.6015652514 | 4.4472449285 | -0.6854142865 |
| H | -0.0290852830 | 4.2081155618 | 0.0018211087 |
| H | 0.3567009895 | 3.5515908018 | -1.6125287460 |
| H | 0.8991841919 | -2.5580896760 | 1.8845888187 |
| H | 0.9435909641 | -3.7456774409 | 0.5645586595 |
| H | 3.3750369225 | -3.6154715842 | 0.1930443683 |
| H | 5.2892571023 | -2.2903908421 | -0.7388989408 |
| H | 4.9321462350 | 0.1394078741 | -1.2454077092 |
| H | 3.5308130497 | 2.1418939978 | -0.9191555970 |
| H | 2.2024965819 | 1.5902720507 | -1.9645355927 |
| H | -4.2253365521 | -0.6847397446 | 2.1493949008 |
| C | -3.5465661949 | -0.1267364229 | 1.5006058616 |
| C | -3.7280402921 | -0.1934115697 | 0.0990822381 |
| H | -4.5344298524 | -0.7902330570 | -0.3310232052 |
| C | -2.8878911888 | 0.5169583421 | -0.7257386206 |
| Cl | -3.1006483228 | 0.4683434292 | -2.4418620218 |

| | | | |
|---|---------------|--------------|---------------|
| C | -1.8579438685 | 1.3573478455 | -0.2045006555 |
| H | -1.4979538694 | 2.1527085907 | -0.8591280552 |
| C | -1.6924103280 | 1.4123853557 | 1.2060274972 |
| H | -1.1717396581 | 2.2552571308 | 1.6667315964 |
| C | -2.5415852017 | 0.6368024365 | 2.0467120778 |
| H | -2.4322912612 | 0.7132629401 | 3.1304301442 |

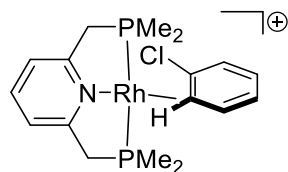


46

Rh-SC-2

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.3021720417 | 0.3888920612 | -0.0969682613 |
| P | 1.7075105555 | 2.1763424881 | 0.0388439796 |
| P | -0.6132547579 | -1.7095710537 | -0.1633414954 |
| N | 2.0357737730 | -0.6605315022 | 0.1030834514 |
| C | 3.0172554278 | 1.3608262642 | 1.0507859680 |
| C | 3.1461475984 | -0.0643399790 | 0.6126860148 |
| C | 4.3469275173 | -0.7572138636 | 0.7378224980 |
| C | 4.4133087743 | -2.0938701151 | 0.3637655530 |
| C | 3.2717898721 | -2.7010077766 | -0.1446035127 |
| C | 2.0993729625 | -1.9626150427 | -0.2808251384 |
| C | 0.8633896014 | -2.5603802638 | -0.8750757307 |
| C | 2.5752066044 | 2.7391083183 | -1.4647393050 |
| H | 3.3940726442 | 3.4321059392 | -1.2197688281 |
| H | 2.9773894550 | 1.8658894673 | -1.9969881679 |
| H | 1.8595920446 | 3.2436791501 | -2.1289646281 |
| C | 1.3159922184 | 3.7151106580 | 0.9328058081 |
| H | 0.8622197122 | 3.4695462831 | 1.9025878584 |
| H | 2.2151202418 | 4.3295440504 | 1.0894054139 |
| H | 0.5877958633 | 4.2954292734 | 0.3480653584 |
| C | -1.9956901063 | -2.2468764106 | -1.2227854355 |
| H | -1.8919458301 | -1.8024261472 | -2.2218776526 |
| H | -2.0199409540 | -3.3437013806 | -1.3066209396 |
| H | -2.9421970409 | -1.9022291497 | -0.7835777996 |
| C | -0.9011948603 | -2.6023232074 | 1.4046106189 |
| H | -1.0436459455 | -3.6788682629 | 1.2263293544 |
| H | -1.7978883920 | -2.1986207146 | 1.8936785344 |
| H | -0.0415066649 | -2.4504593560 | 2.0719287075 |
| H | 3.9864805252 | 1.8813983014 | 1.0270771691 |
| H | 2.6489779417 | 1.3879659688 | 2.0909308736 |
| H | 5.2191918214 | -0.2429258087 | 1.1436484534 |
| H | 5.3441865519 | -2.6552453279 | 0.4661529929 |
| H | 3.2818191509 | -3.7465051047 | -0.4559046380 |
| H | 0.8410573208 | -2.3441319095 | -1.9572322062 |
| H | 0.8444090827 | -3.6539970362 | -0.7536832927 |
| H | -6.0413855980 | -0.1160620330 | -1.3081576860 |
| C | -5.2409029420 | -0.0039976512 | -0.5737753934 |

| | | | |
|----|---------------|---------------|---------------|
| C | -5.3630009516 | -0.5794963338 | 0.6903909686 |
| H | -6.2624290368 | -1.1422817435 | 0.9480575587 |
| C | -4.3430608050 | -0.4277215239 | 1.6312003258 |
| C | -3.1923071005 | 0.2912064754 | 1.3121557278 |
| H | -2.3814386101 | 0.4249824451 | 2.0303665308 |
| C | -3.0932560273 | 0.8418713467 | 0.0394381411 |
| Cl | -1.6338625884 | 1.7262158188 | -0.3877140243 |
| C | -4.0960711863 | 0.7178620292 | -0.9136079892 |
| H | -3.9822809500 | 1.1677843394 | -1.9011802414 |
| H | -4.4460509363 | -0.8644028452 | 2.6272048773 |



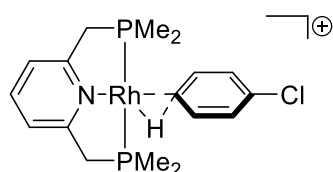
Rh-SC-3

46

Rh-SC-3

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.0928965078 | 0.2729141443 | 0.1163773358 |
| P | -0.3690909839 | -1.9667018182 | -0.0990410561 |
| P | 1.1344685244 | 2.2893699094 | 0.3251795188 |
| N | 2.0184450970 | -0.3916884664 | -0.1382583159 |
| C | 1.0638008140 | -2.3641462854 | -1.1977364312 |
| C | 2.2551591443 | -1.5871790944 | -0.7363667516 |
| C | 3.5527449273 | -2.0574849552 | -0.9224370575 |
| C | 4.6303688645 | -1.2810052782 | -0.5152836421 |
| C | 4.3807656366 | -0.0516997941 | 0.0832339489 |
| C | 3.0671145274 | 0.3672444801 | 0.2730502806 |
| C | 2.7484158867 | 1.6583731216 | 0.9587100952 |
| C | -0.1174971676 | -3.0579762736 | 1.3403103816 |
| H | -0.1019106289 | -4.1151360395 | 1.0357904989 |
| H | 0.8334558663 | -2.8008382972 | 1.8272310892 |
| H | -0.9306088652 | -2.8949612890 | 2.0597102737 |
| C | -1.7970041037 | -2.6835954380 | -0.9738742052 |
| H | -2.0082390723 | -2.0962152154 | -1.8778848832 |
| H | -1.5981927136 | -3.7302750599 | -1.2478568844 |
| H | -2.6778928247 | -2.6487921233 | -0.3191251355 |
| C | 0.6377532450 | 3.5763562988 | 1.5155607892 |
| H | 0.4571115299 | 3.1184058486 | 2.4977329973 |
| H | 1.4089333075 | 4.3554229947 | 1.6080400314 |
| H | -0.2976418932 | 4.0420196945 | 1.1729440271 |
| C | 1.5791271262 | 3.2252209613 | -1.1794233116 |
| H | 2.3004736160 | 4.0242074810 | -0.9507589383 |
| H | 0.6761700818 | 3.6759542598 | -1.6151055250 |
| H | 2.0128408263 | 2.5383716171 | -1.9194223625 |
| H | 1.2825634438 | -3.4407908798 | -1.2618382059 |
| H | 0.7748801683 | -2.0225595254 | -2.2067434049 |
| H | 3.7058011086 | -3.0262200736 | -1.4000313872 |
| H | 5.6545324702 | -1.6298256131 | -0.6626544319 |
| H | 5.1991314216 | 0.5855870533 | 0.4211470213 |

| | | | |
|----|---------------|---------------|---------------|
| H | 2.5938719789 | 1.4674989706 | 2.0348679071 |
| H | 3.5714536197 | 2.3827019550 | 0.8648964465 |
| H | -1.3142332857 | 1.1341139932 | 0.8421752946 |
| C | -2.0935574440 | 0.8473437344 | 0.0456585124 |
| C | -2.2595157392 | 1.5868073142 | -1.1332717634 |
| H | -1.4691678702 | 2.2687972872 | -1.4515106815 |
| C | -3.4145289793 | 1.4472836084 | -1.8986263728 |
| C | -4.4411179480 | 0.6144994764 | -1.4548290131 |
| H | -5.3584300524 | 0.5170227723 | -2.0397040673 |
| C | -4.3239032604 | -0.0792471848 | -0.2501366272 |
| H | -5.1365445470 | -0.7072036029 | 0.1184096481 |
| C | -3.1532473674 | 0.0432478424 | 0.4895513250 |
| Cl | -2.9995926183 | -0.8173650477 | 1.9853862047 |
| H | -3.5245799324 | 2.0062001917 | -2.8297420498 |



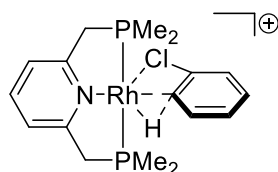
Rh-H-TS

46

Rh-H-TS

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.3259462168 | -0.0677487114 | -0.3187799268 |
| P | 0.2321966852 | 2.2167649535 | -0.3532626834 |
| P | 1.0392826864 | -2.2482932213 | -0.3127781146 |
| N | 2.3480139782 | 0.2831544809 | 0.2621517679 |
| C | 2.0384028885 | 2.5921613534 | -0.4853505931 |
| C | 2.8733476591 | 1.5274825490 | 0.1626752339 |
| C | 4.1691334355 | 1.7931573980 | 0.5995008128 |
| C | 4.9423830801 | 0.7565731913 | 1.1099206704 |
| C | 4.4017065999 | -0.5222385426 | 1.1823965879 |
| C | 3.0901470602 | -0.7327126158 | 0.7633662075 |
| C | 2.4429809658 | -2.0825513418 | 0.8824580534 |
| C | -0.5284457246 | 3.2481784150 | -1.6445118349 |
| H | -0.1923058790 | 4.2916249927 | -1.5526033246 |
| H | -0.2637652807 | 2.8609254548 | -2.6376679135 |
| H | -1.6204150055 | 3.2191924206 | -1.5302042289 |
| C | -0.3063920885 | 2.9820463354 | 1.2106666976 |
| H | 0.2414333668 | 2.5314085115 | 2.0501385636 |
| H | -0.1440648503 | 4.0700535669 | 1.2075676418 |
| H | -1.3767274374 | 2.7702033737 | 1.3476207740 |
| C | 1.8220316058 | -2.7902209271 | -1.8674242661 |
| H | 2.5048690712 | -2.0070802476 | -2.2245281219 |
| H | 2.3769296242 | -3.7298295195 | -1.7275926144 |
| H | 1.0422345151 | -2.9380490183 | -2.6277619712 |
| C | 0.1212912101 | -3.7132021736 | 0.2579540283 |
| H | 0.7522387734 | -4.6126811006 | 0.2079131697 |
| H | -0.7599984005 | -3.8531284244 | -0.3840709040 |
| H | -0.2239096451 | -3.5701891699 | 1.2906034906 |
| H | 2.2633424002 | 2.5974056634 | -1.5667839065 |

| | | | |
|----|---------------|---------------|---------------|
| H | 2.2941333713 | 3.5917378053 | -0.1018315925 |
| H | 4.5694292933 | 2.8048605233 | 0.5199462516 |
| H | 5.9644191359 | 0.9440395175 | 1.4464707995 |
| H | 4.9842713305 | -1.3566538556 | 1.5754680928 |
| H | 3.1856347477 | -2.8893393402 | 0.7844921067 |
| H | 1.9984963953 | -2.1788856874 | 1.8888306431 |
| C | -4.4386236767 | -0.3740619543 | 0.3308266906 |
| C | -3.5220224381 | -1.1110720603 | 1.0791059528 |
| H | -3.8689748942 | -1.7187622975 | 1.9167364897 |
| C | -2.1712211987 | -1.0716728469 | 0.7419973926 |
| C | -1.6974762610 | -0.2666086828 | -0.3083729740 |
| C | -2.6513813104 | 0.4423014955 | -1.0582575692 |
| H | -2.3406817594 | 1.0404541028 | -1.9177103493 |
| C | -4.0089384763 | 0.3956420882 | -0.7470107449 |
| H | -4.7356632179 | 0.9520603682 | -1.3414918414 |
| H | -0.5547604362 | -0.4227041084 | -1.5189547787 |
| Cl | -6.1203697261 | -0.4305805439 | 0.7344879545 |
| H | -1.4760630593 | -1.6631402072 | 1.3413152622 |



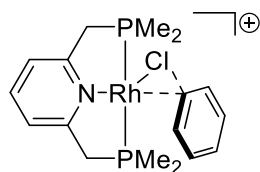
Rh-H-TS'

46

Rh-H-TS'

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.0225154872 | -0.0209935020 | -0.4248325744 |
| P | 0.1467956036 | -2.2819886254 | -0.1771704375 |
| P | -0.7291756352 | 2.1258533162 | -0.7402996289 |
| N | -1.9864476304 | -0.3227253235 | 0.1332599161 |
| C | -1.6481692067 | -2.6944570686 | -0.3530162021 |
| C | -2.5044699578 | -1.5743532710 | 0.1596716864 |
| C | -3.8021542302 | -1.7990859285 | 0.6123762101 |
| C | -4.5816273118 | -0.7191377114 | 1.0122442909 |
| C | -4.0448037813 | 0.5621760560 | 0.9642577342 |
| C | -2.7317701835 | 0.7361623353 | 0.5325281781 |
| C | -2.0834474593 | 2.0897605120 | 0.5178169044 |
| C | 0.9983794267 | -3.3979551080 | -1.3322368852 |
| H | 0.7304196222 | -4.4463952065 | -1.1345193262 |
| H | 0.7352142222 | -3.1357583172 | -2.3658276860 |
| H | 2.0827112070 | -3.2768680054 | -1.2025538485 |
| C | 0.6236191343 | -2.8876052849 | 1.4738617502 |
| H | 0.0287442813 | -2.3693226535 | 2.2388580658 |
| H | 0.4817717552 | -3.9745393458 | 1.5666829196 |
| H | 1.6819825443 | -2.6396400901 | 1.6400865729 |
| C | -1.5938297877 | 2.4146902637 | -2.3195440493 |
| H | -2.2707230847 | 1.5736443157 | -2.5237386600 |
| H | -2.1668215233 | 3.3536301437 | -2.2933803105 |
| H | -0.8542732751 | 2.4639227860 | -3.1310088158 |
| C | 0.1822493099 | 3.6685242773 | -0.4352075256 |

| | | | |
|----|---------------|---------------|---------------|
| H | -0.4843043311 | 4.5406709055 | -0.5045830138 |
| H | 0.9752531176 | 3.7620715883 | -1.1907625313 |
| H | 0.6512164516 | 3.6284011926 | 0.5561517264 |
| H | -1.8257283111 | -2.8034721540 | -1.4375141506 |
| H | -1.9181600864 | -3.6530761692 | 0.1154799428 |
| H | -4.1983000839 | -2.8152468729 | 0.6340713814 |
| H | -5.6051165281 | -0.8762664759 | 1.3597186980 |
| H | -4.6305339761 | 1.4287452770 | 1.2739579545 |
| H | -2.8272350611 | 2.8889362543 | 0.3783680374 |
| H | -1.5905450946 | 2.2648641511 | 1.4902227939 |
| H | 5.8883491360 | 0.1244670121 | 0.6179456525 |
| C | 4.8314980699 | 0.1096618594 | 0.3445252066 |
| C | 3.8905149515 | 0.6914904699 | 1.1909270986 |
| H | 4.1899568805 | 1.1466504469 | 2.1368830776 |
| C | 2.5450682885 | 0.6782848523 | 0.8347970586 |
| Cl | 1.4082401116 | 1.3481815324 | 1.9893460802 |
| C | 2.0788582977 | 0.0856842227 | -0.3534549691 |
| C | 3.0595183458 | -0.4970234922 | -1.1777343073 |
| H | 2.7512670751 | -0.9539609606 | -2.1215250719 |
| C | 4.4119344780 | -0.4896579526 | -0.8397181185 |
| H | 5.1394734364 | -0.9477810904 | -1.5131247184 |
| H | 1.0990700229 | 0.3867904948 | -1.4645282205 |



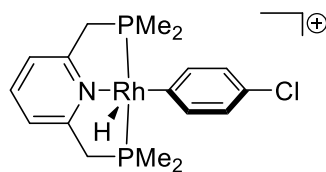
Rh-Cl-TS

46

Rh-Cl-TS

| | | | |
|----|---------------|---------------|---------------|
| Rh | -0.1199999619 | -0.0493190752 | -0.5791059514 |
| P | 0.6457235243 | -2.2253516184 | -0.6223980851 |
| P | -0.0551598592 | 2.2523504353 | -0.5677034710 |
| N | 1.6968324335 | 0.1848131840 | 0.3854239658 |
| C | 1.5103030740 | -2.1603159644 | 1.0091035341 |
| C | 2.2351855317 | -0.8525149228 | 1.0759946508 |
| C | 3.4279230112 | -0.7038346498 | 1.7788962617 |
| C | 4.0812244484 | 0.5227985640 | 1.7683048014 |
| C | 3.5467357823 | 1.5646350526 | 1.0177161870 |
| C | 2.3613308268 | 1.3665557361 | 0.3165318350 |
| C | 1.7840276180 | 2.4121389946 | -0.5846174903 |
| C | -0.2165960434 | -3.8315975267 | -0.6652617139 |
| H | 0.5144317685 | -4.6475064939 | -0.7601367307 |
| H | -0.8045361281 | -3.9924187147 | 0.2472684023 |
| H | -0.8940407990 | -3.8544856787 | -1.5308432266 |
| C | 1.9820232599 | -2.4485567434 | -1.8464918539 |
| H | 2.6546468809 | -1.5803944296 | -1.8230158111 |
| H | 2.5568954635 | -3.3662655609 | -1.6516097131 |
| H | 1.5346692544 | -2.5071665719 | -2.8490216089 |
| C | -0.4943427457 | 3.2242005695 | 0.9149092106 |

| | | | |
|----|---------------|---------------|---------------|
| H | -0.0948295316 | 2.7211016002 | 1.8067877183 |
| H | -0.0740166530 | 4.2385463057 | 0.8444657804 |
| H | -1.5833485953 | 3.2920788534 | 1.0234094925 |
| C | -0.6459819309 | 3.2473586624 | -1.9707139219 |
| H | -0.3108843826 | 4.2920859013 | -1.8934382562 |
| H | -1.7449186137 | 3.2232706035 | -1.9880093518 |
| H | -0.2827900744 | 2.8050921961 | -2.9082305994 |
| H | 0.7092088263 | -2.1892389896 | 1.7690576622 |
| H | 2.1900066785 | -3.0052417221 | 1.1949998048 |
| H | 3.8330297848 | -1.5525347358 | 2.3316288687 |
| H | 5.0106509223 | 0.6605982934 | 2.3247843376 |
| H | 4.0521112465 | 2.5292879023 | 0.9549111348 |
| H | 2.1357018650 | 3.4201474134 | -0.3199160775 |
| H | 2.1076964688 | 2.2059929412 | -1.6197703991 |
| H | -3.0493700794 | -2.3049423908 | 2.7499274613 |
| C | -2.9644698089 | -1.3906375749 | 2.1576578956 |
| C | -2.2977120055 | -1.4363876359 | 0.9333301475 |
| H | -1.9230113348 | -2.3803991352 | 0.5477889252 |
| C | -2.1509497357 | -0.2583474213 | 0.1922124675 |
| Cl | -2.0638424762 | -0.4303398683 | -1.8244766612 |
| C | -2.8310992052 | 0.9045790375 | 0.5803064060 |
| H | -2.8562106368 | 1.7672122698 | -0.0860918802 |
| C | -3.4987625792 | 0.9299917399 | 1.7992044565 |
| H | -4.0086026732 | 1.8455559110 | 2.1090142503 |
| C | -3.5482755759 | -0.2083215584 | 2.6069191042 |
| H | -4.0826883696 | -0.1849884177 | 3.5582525450 |



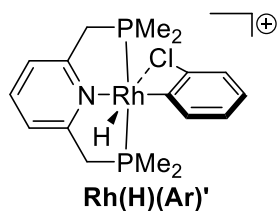
Rh(H)(Ar)

46

Rh(H)(Ar)

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.3102746550 | -0.0058545867 | -0.0663548851 |
| P | 0.5160167137 | 2.2596578553 | -0.0447230941 |
| P | 0.6670476203 | -2.2667252674 | -0.2417440261 |
| N | 2.4504992026 | 0.0400441747 | 0.1417452879 |
| C | 2.3187914195 | 2.4179230899 | -0.4379126087 |
| C | 3.1110799558 | 1.2062289568 | -0.0230634926 |
| C | 4.4964286075 | 1.2647326034 | 0.1189432625 |
| C | 5.2012241362 | 0.0973162886 | 0.3921257267 |
| C | 4.5095266016 | -1.1023262159 | 0.5241815013 |
| C | 3.1210687656 | -1.1025197010 | 0.4060550620 |
| C | 2.3154688029 | -2.3591789622 | 0.6067502455 |
| C | -0.3448843692 | 3.3352179656 | -1.2253227661 |
| H | -0.0143156799 | 4.3798820965 | -1.1337228481 |
| H | -0.1665323714 | 2.9769698801 | -2.2482707229 |
| H | -1.4233228944 | 3.2728201650 | -1.0210033434 |
| C | 0.2953881401 | 3.0623669116 | 1.5766328881 |

| | | | |
|----|---------------|---------------|---------------|
| H | 0.8936829605 | 2.5394853646 | 2.3362284427 |
| H | 0.5999521319 | 4.1189305142 | 1.5396985964 |
| H | -0.7644335612 | 2.9994850691 | 1.8623459868 |
| C | 0.9493863593 | -2.9281817570 | -1.9123895403 |
| H | 1.6845997913 | -2.2997939890 | -2.4336212316 |
| H | 1.3134100384 | -3.9652918841 | -1.8721195375 |
| H | 0.0038493398 | -2.8946080398 | -2.4717926907 |
| C | -0.3718620678 | -3.5045394273 | 0.5904063653 |
| H | 0.0547475331 | -4.5144374418 | 0.5033037887 |
| H | -1.3684226703 | -3.4857426027 | 0.1265451083 |
| H | -0.4862924925 | -3.2437083039 | 1.6513684858 |
| H | 2.3787432360 | 2.5040526911 | -1.5376009523 |
| H | 2.7561003989 | 3.3412352387 | -0.0281263701 |
| H | 5.0158437918 | 2.2163519017 | -0.0045392769 |
| H | 6.2882497149 | 0.1211477067 | 0.4953300502 |
| H | 5.0377309466 | -2.0342291990 | 0.7316452028 |
| H | 2.8900922419 | -3.2504907279 | 0.3112095674 |
| H | 2.0957228057 | -2.4724542861 | 1.6835782003 |
| C | -4.4853439944 | -0.0440186832 | 0.1461036640 |
| C | -3.6881371155 | -0.4375848179 | 1.2188367434 |
| H | -4.1519172139 | -0.7411036968 | 2.1591171091 |
| C | -2.3017912358 | -0.4463833824 | 1.0647317966 |
| C | -1.6855564048 | -0.0480808753 | -0.1327910727 |
| C | -2.5184693777 | 0.3407129693 | -1.1919823465 |
| H | -2.0884850707 | 0.6523350393 | -2.1474861435 |
| C | -3.9073300293 | 0.3400327630 | -1.0621586739 |
| H | -4.5458279543 | 0.6406878722 | -1.8950260962 |
| H | 0.3297898636 | 0.0740689560 | -1.5672574718 |
| Cl | -6.2110903335 | -0.0364915267 | 0.3162649586 |
| H | -1.6961772842 | -0.7763843651 | 1.9195709393 |

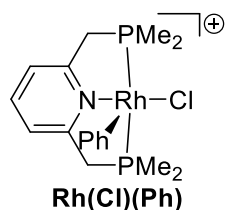


46

Rh(H)(Ar)'

| | | | |
|----|---------------|---------------|---------------|
| H | -0.0881399767 | 0.1262491999 | 1.7765178579 |
| Rh | 0.0719579578 | 0.0291879584 | 0.2695637209 |
| P | -0.1669253995 | -2.2401533595 | 0.4444272526 |
| P | -0.2585247686 | 2.2823321859 | 0.2370523410 |
| N | -2.0375166802 | -0.0427310026 | -0.0480339213 |
| C | -1.7140143152 | -2.4082140734 | -0.5637340267 |
| C | -2.6138383572 | -1.2141960666 | -0.3924378564 |
| C | -3.9868143833 | -1.2914162125 | -0.6187406267 |
| C | -4.7571611365 | -0.1380983496 | -0.5136663223 |
| C | -4.1462810528 | 1.0615401311 | -0.1637642614 |
| C | -2.7749104251 | 1.0799292713 | 0.0843029814 |
| C | -2.0799387356 | 2.3231786237 | 0.5697810597 |

| | | | |
|----|---------------|---------------|---------------|
| C | 1.0241975180 | -3.3971359676 | -0.2900804254 |
| H | 0.6354357040 | -4.4256286899 | -0.3052868034 |
| H | 1.2651599034 | -3.0704398015 | -1.3108906236 |
| H | 1.9469546599 | -3.3641740975 | 0.3064309544 |
| C | -0.5792018044 | -2.9368014732 | 2.0728692964 |
| H | -1.3981926265 | -2.3552571333 | 2.5182252518 |
| H | -0.8773907178 | -3.9921628969 | 1.9895850943 |
| H | 0.2991851872 | -2.8567958841 | 2.7284502432 |
| C | -0.0219090453 | 3.1523829609 | -1.3440527928 |
| H | -0.5697085070 | 2.6282029658 | -2.1390496102 |
| H | -0.3668798036 | 4.1950668272 | -1.2818598355 |
| H | 1.0478043528 | 3.1354610387 | -1.5968977873 |
| C | 0.4920125982 | 3.3636135884 | 1.4871397412 |
| H | 0.1043935655 | 4.3906059648 | 1.4232041998 |
| H | 1.5788918567 | 3.3728934287 | 1.3221607664 |
| H | 0.2999357599 | 2.9531589168 | 2.4875590933 |
| H | -1.3752005217 | -2.4480240600 | -1.6145962671 |
| H | -2.2531982898 | -3.3473886849 | -0.3669672899 |
| H | -4.4398937096 | -2.2462481766 | -0.8895395965 |
| H | -5.8326040062 | -0.1746617490 | -0.7004704090 |
| H | -4.7285736189 | 1.9788290124 | -0.0639865290 |
| H | -2.5608698160 | 3.2313102110 | 0.1758058111 |
| H | -2.1788099668 | 2.3637539383 | 1.6692109302 |
| H | 5.1342473661 | 0.2937068012 | 1.8339124792 |
| C | 4.3930833697 | 0.1978703514 | 1.0368120100 |
| C | 3.0315055617 | 0.2031532221 | 1.3582020985 |
| H | 2.7231066426 | 0.3022821278 | 2.4023374122 |
| C | 2.0675987962 | 0.0794002405 | 0.3519473084 |
| C | 2.5538431496 | -0.0421421865 | -0.9468518541 |
| Cl | 1.2395662719 | -0.1886945932 | -2.1486539142 |
| C | 3.8879122195 | -0.0536921846 | -1.3173403975 |
| H | 4.1920589835 | -0.1534010887 | -2.3609536211 |
| C | 4.8215553418 | 0.0705042194 | -0.2855727259 |
| H | 5.8876455944 | 0.0673484135 | -0.5213385600 |

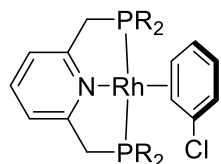


46

Rh(Cl)(Ph)

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.2089899715 | -0.1921974227 | -0.7231371087 |
| P | -0.9653975184 | -2.1541580724 | -0.4424522762 |
| P | 1.0538769958 | 1.9369028196 | -0.8532066831 |
| N | -1.4499517855 | 0.7213872862 | 0.0636630798 |
| C | -2.6515412468 | -1.4020990585 | -0.2970608611 |
| C | -2.6067776171 | 0.0229704776 | 0.1834069275 |
| C | -3.7497510803 | 0.6295807502 | 0.6998043807 |
| C | -3.7124653457 | 1.9694113159 | 1.0655462134 |

| | | | |
|----|---------------|---------------|---------------|
| C | -2.5239385749 | 2.6755155468 | 0.9214289219 |
| C | -1.3923520156 | 2.0268857102 | 0.4347217847 |
| C | -0.0666511317 | 2.7298376010 | 0.3769846886 |
| C | -1.0612367053 | -3.3283749883 | -1.8215416816 |
| H | -1.8146485404 | -4.1074413635 | -1.6353157087 |
| H | -1.2944623235 | -2.7914161350 | -2.7508346699 |
| H | -0.0705560601 | -3.7893606181 | -1.9409690398 |
| C | -0.7036343485 | -3.1646011333 | 1.0422913889 |
| H | -0.7645276792 | -2.5358916144 | 1.9399287024 |
| H | -1.4442421292 | -3.9757006792 | 1.0934800732 |
| H | 0.3087589659 | -3.5907666498 | 0.9959505184 |
| C | 0.7813522167 | 2.7859822093 | -2.4369966840 |
| H | -0.2734436395 | 2.6926652789 | -2.7318238409 |
| H | 1.0504144118 | 3.8504594398 | -2.3706756457 |
| H | 1.4008073720 | 2.2957926522 | -3.2018577217 |
| C | 2.7472725331 | 2.3280352390 | -0.3506409348 |
| H | 2.9174936843 | 3.4142217832 | -0.3380733579 |
| H | 3.4316648732 | 1.8562648832 | -1.0701486440 |
| H | 2.9380873623 | 1.9016995260 | 0.6434763072 |
| H | -4.6669081846 | 0.0467537842 | 0.7971821216 |
| H | -4.6039678939 | 2.4603002123 | 1.4614887157 |
| H | -2.4581088060 | 3.7269339285 | 1.2046177522 |
| H | -0.1932373254 | 3.8114010287 | 0.2231552835 |
| H | 0.4330822694 | 2.5937995813 | 1.3530945819 |
| H | 4.0147209806 | -1.2651817113 | 2.4363266298 |
| C | 2.9735051458 | -0.9346258868 | 2.4045108821 |
| C | 2.2865658348 | -0.6655791101 | 3.5868438132 |
| H | 2.7823612894 | -0.7792990603 | 4.5529792533 |
| C | 0.9585561273 | -0.2557721161 | 3.5204594471 |
| H | 0.4003892113 | -0.0472081850 | 4.4367325702 |
| C | 0.3187568193 | -0.1102479382 | 2.2855766679 |
| H | -0.7280380126 | 0.1945464582 | 2.2832110290 |
| C | 1.0130021123 | -0.3702933265 | 1.0981419742 |
| C | 2.3482607410 | -0.7904127347 | 1.1645220789 |
| H | 2.9005620102 | -1.0093387755 | 0.2507970615 |
| H | -3.3342215422 | -2.0017379415 | 0.3239846981 |
| H | -3.0745602437 | -1.4101233826 | -1.3175662284 |
| Cl | 1.8018532835 | -1.1100735516 | -2.1301862442 |



(tBuL1)Rh-SC-1

R = tBu

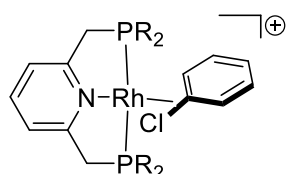
82

(tBuL1)Rh-SC-1

| | | | |
|----|---------------|---------------|--------------|
| Rh | -0.1114988113 | -0.1126675083 | 0.1431065767 |
| P | 2.1484575552 | 0.6360635923 | 0.2290684847 |
| P | -2.4523304048 | -0.0662181932 | 0.0555721979 |

| | | | |
|----|---------------|---------------|---------------|
| N | -0.4124733952 | 1.8494048842 | -0.5808097721 |
| C | 1.7356190274 | 2.4375688605 | 0.3619318577 |
| C | 0.5254758912 | 2.8058384261 | -0.4104288187 |
| C | 0.3506482639 | 4.1035909175 | -0.8904705323 |
| C | -0.8259278524 | 4.4405020104 | -1.5435381789 |
| C | -1.8006334906 | 3.4618035260 | -1.6960218023 |
| C | -1.5669037628 | 2.1787142868 | -1.2100136201 |
| C | -2.5787900060 | 1.1020429323 | -1.3675285490 |
| C | 3.2836237505 | 0.5160942574 | 1.7538719366 |
| C | 3.1345420721 | 0.5533661328 | -1.3873534068 |
| C | -3.1488416252 | 0.8718234515 | 1.5570923990 |
| C | -3.6379153600 | -1.4477552353 | -0.5006772121 |
| H | 1.5158300288 | 2.6056750212 | 1.4294223093 |
| H | 2.5823849835 | 3.0881657132 | 0.1069958893 |
| H | 1.1392539262 | 4.8403919136 | -0.7321747703 |
| H | -0.9853757434 | 5.4518162063 | -1.9232574081 |
| H | -2.7444879070 | 3.6785348135 | -2.1979846770 |
| H | -3.5845759283 | 1.5113506333 | -1.5325982474 |
| H | -2.3116356349 | 0.5023702316 | -2.2512008853 |
| H | 2.7479894055 | -3.7081032459 | 2.1512770596 |
| C | 1.9621323540 | -3.2857575831 | 1.5212317033 |
| C | 2.0186239517 | -3.4944595402 | 0.1244164948 |
| H | 2.8377302903 | -4.0605566410 | -0.3218722682 |
| C | 0.9972408884 | -3.0205686174 | -0.6623907879 |
| Cl | 0.9578293837 | -3.3634850640 | -2.3599788830 |
| C | -0.1115371530 | -2.3231885135 | -0.1130359166 |
| H | -1.0141892040 | -2.3344095254 | -0.7167776250 |
| C | -0.1465734256 | -2.1055740025 | 1.2873316290 |
| H | -1.0894978540 | -1.8850887532 | 1.7906178506 |
| C | 0.9133237100 | -2.6017532712 | 2.0916653385 |
| H | 0.8461442016 | -2.5123227887 | 3.1776103738 |
| C | -4.3038290755 | 1.8061624799 | 1.1943712306 |
| H | -4.6431304858 | 2.3224633106 | 2.1067017916 |
| H | -3.9896803054 | 2.5855315652 | 0.4849439230 |
| H | -5.1701770355 | 1.2819745388 | 0.7744022683 |
| C | -2.0156066979 | 1.7165310558 | 2.1579441423 |
| H | -1.7240049326 | 2.5509068526 | 1.5066097827 |
| H | -2.3682607164 | 2.1504381697 | 3.1072024585 |
| H | -1.1170161010 | 1.1118162068 | 2.3612170279 |
| C | -3.5877685867 | -0.1330940912 | 2.6253956780 |
| H | -4.4687807410 | -0.7165034545 | 2.3300803922 |
| H | -2.7795556102 | -0.8314867477 | 2.8923076111 |
| H | -3.8545056149 | 0.4166526760 | 3.5415574766 |
| C | -5.0985679135 | -0.9895246411 | -0.5043575543 |
| H | -5.4957749970 | -0.8321688473 | 0.5064872775 |
| H | -5.2512254485 | -0.0700976409 | -1.0873287021 |
| H | -5.7109749594 | -1.7760684037 | -0.9731744595 |
| C | -3.2659124536 | -1.8302151671 | -1.9432055541 |
| H | -3.7458216133 | -2.7902254818 | -2.1877897892 |
| H | -3.6344136876 | -1.0941189904 | -2.6709386428 |
| H | -2.1856053512 | -1.9536172463 | -2.1113604418 |
| C | -3.5083974347 | -2.6876883365 | 0.3938335389 |

| | | | |
|---|---------------|---------------|---------------|
| H | -4.2419037002 | -3.4372880321 | 0.0575752629 |
| H | -2.5192399043 | -3.1569694764 | 0.3329434313 |
| H | -3.7224874607 | -2.4776287359 | 1.4484415925 |
| C | 2.3467647867 | 0.3727480524 | 2.9565442816 |
| H | 1.6423767724 | 1.2153673069 | 3.0387295242 |
| H | 1.7578076913 | -0.5476341645 | 2.9014756753 |
| H | 2.9426592363 | 0.3530769835 | 3.8828862144 |
| C | 4.1446273776 | 1.7662102197 | 1.9701892037 |
| H | 4.7860076182 | 2.0063241128 | 1.1143709892 |
| H | 3.5514497006 | 2.6556967530 | 2.2211691320 |
| H | 4.8067503299 | 1.5780017194 | 2.8303697625 |
| C | 4.2071066795 | -0.6972665634 | 1.6598077970 |
| H | 3.6636408593 | -1.6120446645 | 1.3979064297 |
| H | 5.0083510384 | -0.5441883950 | 0.9236398214 |
| H | 4.6894735976 | -0.8605554542 | 2.6366026027 |
| C | 3.5442923379 | -0.8904398572 | -1.6732063554 |
| H | 2.6686050430 | -1.5389624523 | -1.7772319854 |
| H | 4.0896615157 | -0.9214647364 | -2.6296668605 |
| H | 4.2022682217 | -1.3112763920 | -0.9037759790 |
| C | 2.1698742236 | 0.9958685566 | -2.4941442219 |
| H | 1.2362102965 | 0.4125631121 | -2.4685305643 |
| H | 1.9162068861 | 2.0640097434 | -2.4323429823 |
| H | 2.6495555007 | 0.8297901414 | -3.4715016539 |
| C | 4.3756663895 | 1.4439683752 | -1.4058545625 |
| H | 4.8043609089 | 1.4291761405 | -2.4205589500 |
| H | 4.1592129416 | 2.4949837977 | -1.1653954249 |
| H | 5.1558103801 | 1.0831686340 | -0.7225232945 |



(tBuL1)Rh-SC-2

R = tBu

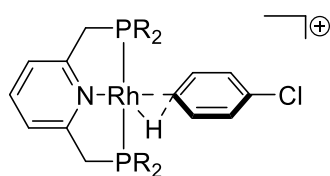
82

(tBuL1)Rh-SC-2

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.0119317143 | -0.1862918546 | 0.1279565347 |
| P | -2.2196424778 | -0.7669086223 | 0.2241101057 |
| P | 2.3317617119 | -0.1951739314 | 0.0525102904 |
| N | 0.2371874127 | -2.0260941417 | -0.7310797279 |
| C | -1.9854864789 | -2.5959384776 | 0.1079033251 |
| C | -0.7589189898 | -2.9451442078 | -0.6665293424 |
| C | -0.6286117622 | -4.2032983143 | -1.2509550149 |
| C | 0.5554057311 | -4.5500416361 | -1.8870982974 |
| C | 1.5850544958 | -3.6186811467 | -1.9209259008 |
| C | 1.4013470916 | -2.3643744466 | -1.3448478351 |
| C | 2.4771987430 | -1.3333162554 | -1.3987083385 |
| C | -3.1388821237 | -0.5901972597 | 1.8653494547 |
| C | -3.2910943617 | -0.3337852568 | -1.2673277198 |
| C | 3.0573665335 | -1.1659394998 | 1.5138291849 |

| | | | |
|----|---------------|---------------|---------------|
| C | 3.4338505969 | 1.2660478427 | -0.4303339285 |
| H | -1.8330973841 | -2.9345745602 | 1.1459874683 |
| H | -2.8661000517 | -3.1334345249 | -0.2723602580 |
| H | -1.4581038654 | -4.9085822980 | -1.1830868475 |
| H | 0.6772013012 | -5.5346794238 | -2.3429952748 |
| H | 2.5367629140 | -3.8481909735 | -2.4020080434 |
| H | 3.4670968387 | -1.7927220950 | -1.5253909835 |
| H | 2.2969365328 | -0.6967008131 | -2.2785900964 |
| H | -0.6346987839 | 4.6864310169 | 1.7075182037 |
| C | -0.5736507443 | 4.5252271449 | 0.6298901286 |
| C | -0.4107342821 | 3.2462957092 | 0.1105932089 |
| Cl | -0.2983591944 | 1.9036540093 | 1.2423821085 |
| C | -0.3244106058 | 2.9950323912 | -1.2523894476 |
| H | -0.2008310880 | 1.9638512800 | -1.5956562404 |
| C | -0.4049471879 | 4.0747045586 | -2.1304631968 |
| H | -0.3401099470 | 3.8982250992 | -3.2064203677 |
| C | -0.5681111349 | 5.3693859961 | -1.6396495443 |
| H | -0.6303412037 | 6.2114780910 | -2.3317168012 |
| C | -0.6525671997 | 5.5911296931 | -0.2649870264 |
| H | -0.7804107629 | 6.6047502079 | 0.1207434234 |
| C | 3.0460547348 | 1.6797281383 | -1.8549854318 |
| H | 3.4719939022 | 2.6731505252 | -2.0647190973 |
| H | 3.4431862692 | 0.9920408882 | -2.6149262764 |
| H | 1.9568161666 | 1.7578246970 | -1.9811199042 |
| C | 4.9267137711 | 0.9409596262 | -0.4065026028 |
| H | 5.4838840354 | 1.7999939527 | -0.8132030420 |
| H | 5.3029979710 | 0.7646992265 | 0.6095896778 |
| H | 5.1763178627 | 0.0681594312 | -1.0280286233 |
| C | 3.3390729954 | -0.1934064056 | 2.6616168900 |
| H | 4.1793076613 | 0.4806385323 | 2.4486864964 |
| H | 2.4546002355 | 0.4158911283 | 2.9049579677 |
| H | 3.6023144847 | -0.7683383748 | 3.5635158600 |
| C | 4.3129833763 | -1.9639137251 | 1.1610905992 |
| H | 5.1445191904 | -1.3389009994 | 0.8162669176 |
| H | 4.6568415084 | -2.5014591208 | 2.0594448125 |
| H | 4.1093881315 | -2.7251932746 | 0.3938155414 |
| C | 1.9794825962 | -2.1524206898 | 1.9820505590 |
| H | 2.3298010767 | -2.6502772789 | 2.9003836999 |
| H | 1.0283021835 | -1.6399313230 | 2.1947288532 |
| H | 1.7832905626 | -2.9370574838 | 1.2378038047 |
| C | -2.0809190146 | -0.7551553221 | 2.9635656431 |
| H | -1.3228319246 | 0.0388235128 | 2.9306951331 |
| H | -2.5740395505 | -0.7137089322 | 3.9477984315 |
| H | -1.5557245825 | -1.7205607379 | 2.9021158130 |
| C | -3.7621896767 | 0.8030749675 | 1.9728970985 |
| H | -3.0424776728 | 1.6007569803 | 1.7385311449 |
| H | -4.6339345324 | 0.9149709015 | 1.3139858529 |
| H | -4.1127790430 | 0.9618906743 | 3.0049378768 |
| C | -4.2211588304 | -1.6547649639 | 2.0638134683 |
| H | -4.7164024827 | -1.4803756457 | 3.0324066385 |
| H | -4.9961030438 | -1.6222675711 | 1.2892818808 |
| H | -3.8093600296 | -2.6735516623 | 2.0956820448 |

| | | | |
|---|---------------|---------------|---------------|
| C | -3.4301990524 | 1.1870195303 | -1.3646588094 |
| H | -2.4546122106 | 1.6884667398 | -1.3233184562 |
| H | -3.8997137282 | 1.4460357764 | -2.3269970193 |
| H | -4.0591553062 | 1.6060334398 | -0.5701264515 |
| C | -4.6721119163 | -0.9845614044 | -1.2545306418 |
| H | -5.3170483980 | -0.5719431031 | -0.4669983387 |
| H | -5.1718997748 | -0.7904082713 | -2.2171551501 |
| H | -4.6254911833 | -2.0766323839 | -1.1292039213 |
| C | -2.4990729379 | -0.8278245514 | -2.4840595961 |
| H | -1.4797211401 | -0.4112845011 | -2.4950439579 |
| H | -2.4198962864 | -1.9242028524 | -2.5186989574 |
| H | -3.0133345518 | -0.5075152224 | -3.4037469817 |
| C | 3.1342572388 | 2.4438857140 | 0.5023477466 |
| H | 3.7895969947 | 3.2873564387 | 0.2337912187 |
| H | 2.0970558186 | 2.7834313737 | 0.3939684866 |
| H | 3.3099223328 | 2.2122837098 | 1.5597036598 |



(tBuL1)Rh-H-TS

R = tBu

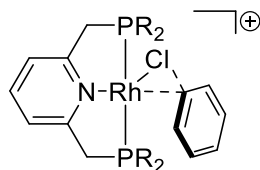
82

(tBuL1)Rh-H-TS

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.2439804725 | 0.0788859077 | -0.0578455330 |
| P | -1.2353595347 | 1.8809526168 | -0.2108033022 |
| P | 2.1930309825 | -1.1873985102 | -0.0447149076 |
| N | 1.5731342206 | 1.5485329230 | 0.6981965080 |
| C | 0.0431275241 | 3.2254575962 | -0.1832476279 |
| C | 1.2655561614 | 2.8587086603 | 0.5917975312 |
| C | 2.1023493143 | 3.8394834948 | 1.1230021369 |
| C | 3.2886167794 | 3.4619379524 | 1.7393281618 |
| C | 3.6158903903 | 2.1120651369 | 1.8065098095 |
| C | 2.7349396752 | 1.1704343930 | 1.2808369753 |
| C | 3.0299910689 | -0.2944513712 | 1.3482357261 |
| C | -2.1415490315 | 2.2533120444 | -1.8262008919 |
| C | -2.2841106129 | 2.2199708715 | 1.3189481409 |
| C | 3.2479461507 | -0.8143126015 | -1.5769282642 |
| C | 2.2697002522 | -3.0106795967 | 0.4415617828 |
| H | -0.3581166740 | 4.1963321951 | 0.1403272870 |
| H | 1.8258195671 | 4.8907112205 | 1.0315756047 |
| H | 3.9604446368 | 4.2157016463 | 2.1557985164 |
| H | 4.5454042962 | 1.7805460333 | 2.2711122536 |
| H | 4.1108816961 | -0.4808022746 | 1.4164957481 |
| H | 2.5761012636 | -0.6977314279 | 2.2668302981 |
| C | -3.4245259481 | -3.0780406702 | 0.2585928296 |
| C | -2.5504990314 | -2.7550716709 | 1.2971631292 |
| H | -2.7103543037 | -3.1733261262 | 2.2925283082 |
| C | -1.4812634940 | -1.8992407009 | 1.0525705483 |

| | | | |
|----|---------------|---------------|---------------|
| C | -1.2672378728 | -1.3196841330 | -0.2128123097 |
| C | -2.1575180420 | -1.6791940148 | -1.2353851943 |
| H | -2.0246309055 | -1.2875866069 | -2.2463923416 |
| C | -3.2271109047 | -2.5475276767 | -1.0110411014 |
| H | -3.9040296183 | -2.8141742574 | -1.8244419212 |
| H | -0.1506838468 | -0.8810498062 | -1.1917712430 |
| Cl | -4.7509307009 | -4.1502183964 | 0.5534588575 |
| H | -0.8225310840 | -1.6535324705 | 1.8888893284 |
| C | 2.9329573739 | 0.6159508665 | -2.0329589370 |
| H | 3.4567070839 | 0.8034728897 | -2.9836887766 |
| H | 1.8537354744 | 0.7625546374 | -2.1909972437 |
| H | 3.2820593232 | 1.3699601224 | -1.3138503837 |
| C | 2.8370187408 | -1.7705640404 | -2.6985083390 |
| H | 3.1217061213 | -2.8104086650 | -2.4934138150 |
| H | 1.7526322076 | -1.7357566871 | -2.8863402124 |
| H | 3.3437604765 | -1.4695603409 | -3.6287519916 |
| C | 4.7506933415 | -0.9077530896 | -1.3082883005 |
| H | 5.0735747102 | -1.9020697231 | -0.9811633511 |
| H | 5.2915250629 | -0.6764398113 | -2.2397380990 |
| H | 5.0784821535 | -0.1717541264 | -0.5595046002 |
| C | 3.6595037610 | -3.6317827518 | 0.3028819712 |
| H | 3.6265263939 | -4.6565165632 | 0.7053855332 |
| H | 3.9872896417 | -3.7069405816 | -0.7421712921 |
| H | 4.4244738312 | -3.0837403825 | 0.8728732217 |
| C | 1.8402486692 | -3.1126750321 | 1.9097684883 |
| H | 1.6422886129 | -4.1694462534 | 2.1462744990 |
| H | 2.6236992209 | -2.7687573985 | 2.6000925212 |
| H | 0.9166574289 | -2.5554124775 | 2.1141778424 |
| C | 1.2583386486 | -3.7778703447 | -0.4187915478 |
| H | 1.2680887905 | -4.8369636828 | -0.1171520390 |
| H | 0.2374475365 | -3.3989563217 | -0.2806165359 |
| H | 1.4968392994 | -3.7403125629 | -1.4888301933 |
| H | 0.3517052549 | 3.3497450379 | -1.2350047163 |
| C | -1.2622637943 | 1.6790570631 | -2.9422162240 |
| H | -1.1690003810 | 0.5879172562 | -2.8706415965 |
| H | -1.7099739382 | 1.9234581091 | -3.9184024195 |
| H | -0.2446267162 | 2.0992652282 | -2.9335448565 |
| C | -3.5077041793 | 1.5652332695 | -1.8421625470 |
| H | -3.4498882430 | 0.5064556086 | -1.5565718172 |
| H | -4.2234779451 | 2.0646489948 | -1.1754921170 |
| H | -3.9221739317 | 1.6176709859 | -2.8612753673 |
| C | -2.3280080077 | 3.7542415598 | -2.0696199276 |
| H | -2.8817996171 | 3.8882060085 | -3.0123543959 |
| H | -2.9074297668 | 4.2456429070 | -1.2787039464 |
| H | -1.3742258323 | 4.2880164236 | -2.1827052350 |
| C | -3.3178872399 | 1.1044810183 | 1.4993281911 |
| H | -2.8525384751 | 0.1111897301 | 1.5281218863 |
| H | -3.8417110540 | 1.2608041281 | 2.4555700941 |
| H | -4.0765702901 | 1.0996625886 | 0.7080402801 |
| C | -2.9864190328 | 3.5759190810 | 1.2929063088 |
| H | -3.7747015803 | 3.6165194130 | 0.5297146707 |
| H | -3.4700344681 | 3.7469114801 | 2.2678151454 |

| | | | |
|---|---------------|--------------|--------------|
| H | -2.2945354156 | 4.4143435429 | 1.1238919403 |
| C | -1.3056804801 | 2.1711521045 | 2.4991281597 |
| H | -0.7424554112 | 1.2249443080 | 2.5209744743 |
| H | -0.5845343724 | 3.0015342172 | 2.4863317654 |
| H | -1.8738479111 | 2.2461706196 | 3.4393884147 |



(tBuL1)Rh-Cl-TS

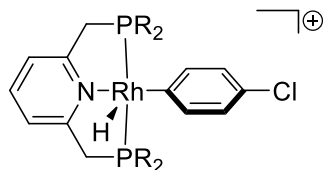
R = tBu

82

(tBuL1)Rh-Cl-TS

| | | | |
|----|---------------|---------------|---------------|
| Rh | 0.0607256832 | 0.1520513017 | 0.2091639656 |
| P | 2.4221788399 | -0.0915411855 | 0.0522723667 |
| P | -2.1867172528 | -0.5158026977 | 0.3711855885 |
| N | 0.1794999273 | -1.5583228761 | -0.9756690994 |
| C | 2.4031851263 | -0.8441903965 | -1.6405530538 |
| C | 1.2677599518 | -1.8026833362 | -1.7436340347 |
| C | 1.3442598600 | -2.9318441331 | -2.5567587346 |
| C | 0.2983056762 | -3.8458204713 | -2.5622025840 |
| C | -0.7709526176 | -3.6373417644 | -1.6991027561 |
| C | -0.7907627353 | -2.5016871377 | -0.8945398426 |
| C | -1.8077562852 | -2.3137459922 | 0.1728150213 |
| C | 3.8374683306 | 1.1923067598 | -0.0790250489 |
| C | 2.9105380270 | -1.4588081955 | 1.2864595657 |
| C | -3.3970673825 | -0.2257131957 | -1.0833049301 |
| C | -3.0437003965 | -0.4812545207 | 2.0547979884 |
| H | 2.2263155911 | 0.0044010643 | -2.3203211194 |
| H | 3.3495175668 | -1.3172901554 | -1.9391271560 |
| H | 2.2300883136 | -3.0848838628 | -3.1745451787 |
| H | 0.3330291506 | -4.7286377273 | -3.2039245835 |
| H | -1.5807998212 | -4.3637179129 | -1.6189326816 |
| H | -2.6887996304 | -2.9467254406 | 0.0193696018 |
| H | -1.3403900672 | -2.6269352057 | 1.1197288564 |
| H | 0.8793466127 | 3.9934631881 | -2.7527785208 |
| C | 0.1374730304 | 3.6542146131 | -2.0255394012 |
| C | 0.5390094988 | 2.8009437904 | -0.9978159088 |
| H | 1.5780067478 | 2.5194591963 | -0.8918466625 |
| C | -0.4054256978 | 2.3163444367 | -0.0926325222 |
| Cl | 0.1569400372 | 1.8940233159 | 1.7789769225 |
| C | -1.7097205736 | 2.8268820678 | -0.1092076151 |
| H | -2.4078320448 | 2.5524982581 | 0.6777288605 |
| C | -2.0900341390 | 3.6985292197 | -1.1224309287 |
| H | -3.1137319609 | 4.0805840243 | -1.1374670627 |
| C | -1.1796234940 | 4.0987869845 | -2.1030863486 |
| H | -1.4863783807 | 4.7855718208 | -2.8938443897 |
| C | -4.4268361894 | 0.8655378510 | -0.7834691971 |
| H | -3.9697160205 | 1.8164870115 | -0.4946394141 |

| | | | |
|---|---------------|---------------|---------------|
| H | -5.0099268992 | 1.0523844967 | -1.6989750518 |
| H | -5.1380022433 | 0.5637563847 | -0.0028692238 |
| C | -4.1634478932 | -1.5003826703 | -1.4548678505 |
| H | -4.7353700623 | -1.9227679296 | -0.6169686960 |
| H | -4.8866165549 | -1.2476846768 | -2.2462107988 |
| H | -3.5076163941 | -2.2799922096 | -1.8665247456 |
| C | -2.5391494450 | 0.1880469439 | -2.2856098940 |
| H | -1.9759100019 | 1.1103704955 | -2.0983283799 |
| H | -1.8232954536 | -0.5972786442 | -2.5672500067 |
| H | -3.1986245614 | 0.3574622070 | -3.1516543358 |
| C | -3.3953454127 | 0.9554326762 | 2.4519158468 |
| H | -2.4939738764 | 1.5782127358 | 2.5353318043 |
| H | -4.1015373624 | 1.4327094832 | 1.7614227059 |
| H | -3.8733820306 | 0.9389013305 | 3.4439235949 |
| C | -4.2955203847 | -1.3583000630 | 2.0792005628 |
| H | -4.7108021313 | -1.3630159498 | 3.0994623077 |
| H | -5.0814297776 | -0.9852987579 | 1.4097216243 |
| H | -4.0810969548 | -2.4036651750 | 1.8133937212 |
| C | -2.0274003351 | -1.0060526314 | 3.0771719507 |
| H | -1.0729377257 | -0.4633064358 | 3.0134864020 |
| H | -2.4354629152 | -0.8582053443 | 4.0890835749 |
| H | -1.8293634054 | -2.0817084604 | 2.9685087706 |
| C | 1.7110338118 | -2.3862167897 | 1.5231107924 |
| H | 1.9601481532 | -3.0599168443 | 2.3579001074 |
| H | 0.8066980851 | -1.8203760344 | 1.7950326385 |
| H | 1.4883629525 | -3.0162492268 | 0.6514826724 |
| C | 3.2082807076 | -0.7725449392 | 2.6247951669 |
| H | 4.1054729844 | -0.1429149331 | 2.6033724928 |
| H | 2.3590172759 | -0.1508400024 | 2.9490855878 |
| H | 3.3692099791 | -1.5433722671 | 3.3946181714 |
| C | 4.0713705893 | -2.3388253038 | 0.8194670640 |
| H | 5.0215813563 | -1.8063654686 | 0.7245278018 |
| H | 4.2208262767 | -3.1441427820 | 1.5563672161 |
| H | 3.8470524717 | -2.8249522048 | -0.1422854311 |
| C | 3.5793195454 | 2.3034156478 | 0.9461451442 |
| H | 4.3909522479 | 3.0450643312 | 0.8820160429 |
| H | 2.6294929465 | 2.8266547891 | 0.7829953974 |
| H | 3.5626931575 | 1.9192837919 | 1.9747405553 |
| C | 5.2309309252 | 0.6055090318 | 0.1668872269 |
| H | 5.9669693146 | 1.4090926212 | 0.0068042482 |
| H | 5.3772196329 | 0.2381658695 | 1.1890744364 |
| H | 5.4757616231 | -0.1998453336 | -0.5395014761 |
| C | 3.8902063740 | 1.7736629906 | -1.5015160667 |
| H | 4.3153180741 | 1.0535240583 | -2.2145127572 |
| H | 2.9293858319 | 2.1115616897 | -1.9071671141 |
| H | 4.5593277653 | 2.6479919769 | -1.4896671904 |



(tBuL1)Rh(H)(Ar)

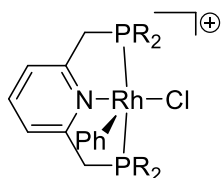
R = tBu

82

(tBuL1)Rh(H)(Ar)

| | | | |
|----|---------------|---------------|---------------|
| H | 0.2462941717 | 0.0411290268 | 1.4904999813 |
| Rh | 0.2679462766 | -0.0467779998 | -0.0037730051 |
| P | 1.1877020692 | 2.0876510955 | -0.0644066060 |
| P | -0.0684479498 | -2.3277808093 | 0.1557745546 |
| N | 2.3395895361 | -0.6193448397 | -0.0763069223 |
| C | 2.8173703521 | 1.6465483832 | -0.8418698334 |
| C | 3.2733718941 | 0.2634288810 | -0.4802566884 |
| C | 4.6126690353 | -0.1114663839 | -0.5871290635 |
| C | 4.9778902966 | -1.4175663426 | -0.2829638277 |
| C | 4.0045299126 | -2.3135836825 | 0.1486507299 |
| C | 2.6852945967 | -1.8799335717 | 0.2608037354 |
| C | 1.6097995514 | -2.7589559105 | 0.8218770386 |
| C | 0.4648384762 | 3.3323321690 | -1.2775959408 |
| C | 1.6431142632 | 2.8243053606 | 1.6077524377 |
| C | -0.1005234191 | -3.1198356486 | -1.5636062417 |
| C | -1.2633254930 | -3.1003898626 | 1.3851882066 |
| H | 2.6480368060 | 1.6847127695 | -1.9308663843 |
| H | 3.6024183775 | 2.3872126686 | -0.6288477398 |
| H | 5.3547949728 | 0.6167771324 | -0.9179016777 |
| H | 6.0191094059 | -1.7348589924 | -0.3727702891 |
| H | 4.2635340969 | -3.3390640002 | 0.4161550040 |
| H | 1.8646175495 | -3.8216552357 | 0.7198894385 |
| H | 1.5474057726 | -2.5492238599 | 1.9021167660 |
| H | -4.2805430220 | 1.6421436570 | 1.9265502371 |
| C | -3.7506322008 | 1.2594261500 | 1.0522424308 |
| C | -2.3912205711 | 0.9527557879 | 1.1221534568 |
| H | -1.8882066910 | 1.1084465138 | 2.0781697306 |
| C | -1.6800689097 | 0.4552436690 | 0.0182961059 |
| C | -2.4133159292 | 0.2741336216 | -1.1678424741 |
| H | -1.9270098393 | -0.1284310549 | -2.0630540941 |
| C | -3.7705476368 | 0.5798756960 | -1.2641890048 |
| H | -4.3138426384 | 0.4305105128 | -2.1991079319 |
| C | -4.4366321820 | 1.0733769056 | -0.1450762073 |
| Cl | -6.1268965667 | 1.4496788165 | -0.2430109517 |
| C | 0.6680465579 | -4.4396232706 | -1.6289815618 |
| H | 0.2846588648 | -5.1889260821 | -0.9234871559 |
| H | 0.5682397450 | -4.8617297132 | -2.6419167355 |
| H | 1.7434246218 | -4.3044382160 | -1.4436906509 |
| C | -1.5407735224 | -3.3332932440 | -2.0323258738 |
| H | -2.0311805497 | -4.1527968601 | -1.4910034318 |
| H | -2.1570818734 | -2.4294826826 | -1.9245463345 |
| H | -1.5291872378 | -3.6079846164 | -3.0989241560 |

| | | | |
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| C | 0.5781708018 | -2.1035096705 | -2.4942370733 |
| H | 0.5207654687 | -2.4636873528 | -3.5338384007 |
| H | 0.0776145214 | -1.1192471188 | -2.4695829036 |
| H | 1.6405557769 | -1.9592719989 | -2.2543643853 |
| C | -0.9743484922 | -2.4522388172 | 2.7443285899 |
| H | -1.0681531710 | -1.3577766538 | 2.6966626363 |
| H | -1.7157006677 | -2.8186489754 | 3.4708512724 |
| H | 0.0172329503 | -2.7065329774 | 3.1448941924 |
| C | -2.7097722421 | -2.7622204699 | 1.0057922252 |
| H | -3.3685579297 | -3.1033176617 | 1.8195226397 |
| H | -2.8612805229 | -1.6818334300 | 0.8812334007 |
| H | -3.0380227043 | -3.2661186926 | 0.0906808544 |
| C | -1.0761574183 | -4.6153017637 | 1.4766042521 |
| H | -1.7411151085 | -5.0136148035 | 2.2589397054 |
| H | -1.3416217671 | -5.1209117786 | 0.5381539386 |
| H | -0.0483919406 | -4.8999030376 | 1.7473420433 |
| C | 0.0309786588 | 2.5060850812 | -2.4940756701 |
| H | -0.7474043928 | 1.7811297886 | -2.2256281311 |
| H | -0.3932564255 | 3.1811900432 | -3.2535683858 |
| H | 0.8682216148 | 1.9739043060 | -2.9728848794 |
| C | 1.4592365306 | 4.4018159638 | -1.7340570338 |
| H | 0.9713417002 | 5.0282430524 | -2.4975343035 |
| H | 1.7771516647 | 5.0665001118 | -0.9231215330 |
| H | 2.3576690027 | 3.9711713657 | -2.2000647577 |
| C | -0.7739888263 | 3.9760188955 | -0.6502104720 |
| H | -1.4895789201 | 3.2210226310 | -0.2916476212 |
| H | -0.5166333945 | 4.6448367465 | 0.1830024665 |
| H | -1.2851558001 | 4.5863633749 | -1.4109629664 |
| C | 0.3887436172 | 2.8859509137 | 2.4823511728 |
| H | -0.0050065802 | 1.8793688586 | 2.6788495437 |
| H | 0.6488954133 | 3.3397965207 | 3.4513269921 |
| H | -0.4169640187 | 3.4832302905 | 2.0367335332 |
| C | 2.2724197256 | 4.2118669569 | 1.4956882275 |
| H | 1.5515958545 | 4.9669349794 | 1.1560348009 |
| H | 2.6264870739 | 4.5232486637 | 2.4909835228 |
| H | 3.1411582690 | 4.2294198655 | 0.8213035772 |
| C | 2.6464654450 | 1.8694081720 | 2.2646691793 |
| H | 2.2622533502 | 0.8404670956 | 2.3213136153 |
| H | 3.6154316054 | 1.8501716135 | 1.7454918180 |
| H | 2.8366483473 | 2.2122040861 | 3.2936486024 |



(tBuL1)Rh(Cl)(Ph)

R = tBu

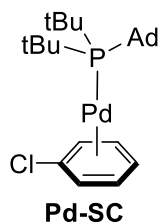
82

(tBuL1)Rh(Cl)(Ph)

| | | | |
|----|---------------|--------------|--------------|
| Rh | -0.0035338822 | 0.1583816586 | 0.3198111972 |
|----|---------------|--------------|--------------|

| | | | |
|----|---------------|---------------|---------------|
| P | 2.3728032790 | 0.3532097464 | 0.1535193309 |
| P | -2.3111370392 | 0.3614584381 | 0.1024085415 |
| N | 0.0086810693 | 0.5683147518 | -1.7068877019 |
| C | 2.3667016903 | 1.2226323497 | -1.4805985713 |
| C | 1.1529658250 | 0.9607730816 | -2.3150043004 |
| C | 1.1795277540 | 1.2277844020 | -3.6838761503 |
| C | 0.0075367419 | 1.1545886906 | -4.4229830554 |
| C | -1.1743087087 | 0.8201623007 | -3.7720132439 |
| C | -1.1500973239 | 0.5182393730 | -2.4136245363 |
| C | -2.3937818185 | 0.0717623174 | -1.7143596047 |
| C | 3.1439609703 | 1.6512202508 | 1.2936262508 |
| C | -2.6645022557 | 2.1994658551 | 0.3654675868 |
| C | -3.6379433225 | -0.7564758338 | 0.8425501301 |
| H | 2.1213734506 | 1.5197095936 | -4.1504544693 |
| H | 0.0105708692 | 1.3713317059 | -5.4932791725 |
| H | -2.1203994716 | 0.7721669393 | -4.3127168676 |
| H | -3.2919545735 | 0.4857010819 | -2.1922515306 |
| H | -2.4520309119 | -1.0245687640 | -1.8091682096 |
| H | -0.3883401032 | -4.6616332489 | 1.8955957972 |
| C | -0.3621858435 | -4.0307283182 | 1.0036571618 |
| C | -0.5001157452 | -4.5982051092 | -0.2611383314 |
| H | -0.6362555859 | -5.6754534550 | -0.3751810458 |
| C | -0.4533900140 | -3.7696844026 | -1.3778951260 |
| H | -0.5444470006 | -4.1920577472 | -2.3817811863 |
| C | -0.2820522252 | -2.3900758832 | -1.2347447484 |
| H | -0.2255163544 | -1.7918061578 | -2.1431944627 |
| C | -0.1604796894 | -1.8129380174 | 0.0355122642 |
| C | -0.1948641578 | -2.6534708104 | 1.1578008054 |
| H | -0.0945065050 | -2.2361368783 | 2.1583388690 |
| H | 3.2868775263 | 1.0524767218 | -2.0576932179 |
| H | 2.3563744192 | 2.2995434189 | -1.2406782275 |
| Cl | -0.0548575210 | 0.1980286284 | 2.6588798019 |
| C | -1.3717649698 | 2.9386767658 | -0.0052488341 |
| H | -1.4974644646 | 4.0112239268 | 0.2130189151 |
| H | -0.5142994612 | 2.6012461194 | 0.6023140450 |
| H | -1.1174621298 | 2.8483335135 | -1.0701744699 |
| C | -3.7956048773 | 2.7369581020 | -0.5105762083 |
| H | -3.5750207240 | 2.6294771241 | -1.5829454472 |
| H | -4.7632805509 | 2.2643282375 | -0.3060101866 |
| H | -3.9103532155 | 3.8149824378 | -0.3135038609 |
| C | -2.9453390868 | 2.4519189213 | 1.8492968071 |
| H | -3.9041960846 | 2.0277181021 | 2.1728165470 |
| H | -2.1476750445 | 2.0427655882 | 2.4874323779 |
| H | -2.9944672284 | 3.5389668060 | 2.0195263119 |
| C | -5.0366628353 | -0.1710585921 | 0.6387376463 |
| H | -5.2658047499 | 0.0029039674 | -0.4233152353 |
| H | -5.7726894098 | -0.8991615548 | 1.0138247723 |
| H | -5.1947995258 | 0.7630572579 | 1.1918348933 |
| C | -3.3391942504 | -0.9417454908 | 2.3322855749 |
| H | -4.1009228582 | -1.6112946392 | 2.7610367854 |
| H | -2.3505556207 | -1.3891684541 | 2.4913372908 |
| H | -3.3676412535 | 0.0006824145 | 2.8918909990 |

| | | | |
|---|---------------|---------------|---------------|
| C | -3.5930679435 | -2.1259122776 | 0.1539971029 |
| H | -3.9476355109 | -2.0848579698 | -0.8859236228 |
| H | -2.5987510535 | -2.5865722211 | 0.1761971096 |
| H | -4.2790708514 | -2.7951630994 | 0.6956263153 |
| C | 2.0796122691 | 2.7304851394 | 1.5202962599 |
| H | 1.7633682608 | 3.2167687175 | 0.5835846856 |
| H | 1.2002432572 | 2.3280245190 | 2.0408362507 |
| H | 2.5098302330 | 3.5211649356 | 2.1545721448 |
| C | 4.3831235332 | 2.3247131533 | 0.6969668238 |
| H | 4.1750486335 | 2.8340932669 | -0.2555437302 |
| H | 4.7228921593 | 3.1000757548 | 1.4018727564 |
| H | 5.2206379469 | 1.6373726240 | 0.5432090748 |
| C | 3.4831518263 | 0.9957716506 | 2.6345764429 |
| H | 2.6190488465 | 0.4562616442 | 3.0481400826 |
| H | 4.3344103154 | 0.3061338342 | 2.5555735680 |
| H | 3.7659396197 | 1.7805295345 | 3.3535165108 |
| C | 4.9715397689 | -0.7803106592 | -0.1974060275 |
| H | 5.5320960078 | -1.6945883056 | -0.4484979079 |
| H | 5.1740217144 | -0.0494056123 | -0.9948022709 |
| H | 5.3833541247 | -0.3980285916 | 0.7450156880 |
| C | 3.4915566814 | -1.1457396036 | -0.0877701618 |
| C | 3.2744299319 | -2.1043610452 | 1.0862361270 |
| H | 3.8944710156 | -3.0012801411 | 0.9318061872 |
| H | 3.5622454220 | -1.6628389252 | 2.0486613674 |
| H | 2.2281851471 | -2.4251205182 | 1.1551289816 |
| C | 3.0668029771 | -1.8302849608 | -1.3899151003 |
| H | 3.2573911070 | -1.2066697240 | -2.2757237233 |
| H | 3.6620666620 | -2.7489592044 | -1.5090245411 |
| H | 2.0117047290 | -2.1249035207 | -1.3804210255 |

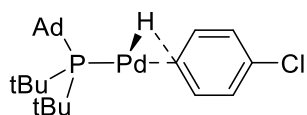


65

Pd-SC

| | | | |
|---|-----------|-----------|-----------|
| P | -0.573296 | -1.209615 | 0.085261 |
| C | -1.453366 | -2.656565 | -0.835083 |
| C | -0.350596 | -1.717356 | 1.933760 |
| C | -2.625254 | -3.319613 | -0.091527 |
| H | -3.071454 | -4.087525 | -0.735860 |
| H | -2.306810 | -3.817190 | 0.825920 |
| H | -3.412373 | -2.608303 | 0.164590 |
| C | -1.956179 | -2.153372 | -2.202506 |
| H | -1.157768 | -1.654212 | -2.758570 |
| H | -2.284516 | -3.017893 | -2.791595 |
| H | -2.806115 | -1.475099 | -2.122607 |
| C | -0.381055 | -3.720424 | -1.161899 |
| H | -0.828100 | -4.486297 | -1.807752 |

| | | | |
|----|-----------|-----------|-----------|
| H | 0.459826 | -3.265013 | -1.694036 |
| H | 0.012329 | -4.223046 | -0.280774 |
| C | 0.735098 | -0.804988 | 2.550948 |
| H | 0.441153 | 0.240150 | 2.616296 |
| H | 0.948092 | -1.155132 | 3.568823 |
| H | 1.656431 | -0.853606 | 1.963710 |
| C | -1.620448 | -1.672033 | 2.800975 |
| H | -2.012732 | -0.660059 | 2.912361 |
| H | -2.418558 | -2.301411 | 2.404055 |
| H | -1.381241 | -2.037861 | 3.807376 |
| C | 0.237954 | -3.140460 | 1.995005 |
| H | -0.477692 | -3.912615 | 1.710638 |
| H | 1.125395 | -3.228936 | 1.361907 |
| H | 0.542674 | -3.346284 | 3.027811 |
| Pd | 1.498802 | -0.682333 | -0.798858 |
| C | -1.698798 | 0.345314 | 0.009539 |
| C | -1.193695 | 1.378442 | 1.050398 |
| C | -3.209880 | 0.115027 | 0.241046 |
| C | -1.495395 | 1.006022 | -1.384779 |
| H | -1.321451 | 0.994228 | 2.063507 |
| H | -0.125097 | 1.557892 | 0.895479 |
| C | -1.969549 | 2.705075 | 0.947469 |
| H | -3.384945 | -0.331374 | 1.224115 |
| H | -3.610660 | -0.580632 | -0.500660 |
| C | -3.982632 | 1.447384 | 0.135487 |
| H | -0.424558 | 1.188422 | -1.529587 |
| H | -1.809606 | 0.337717 | -2.185493 |
| C | -2.286068 | 2.322699 | -1.497253 |
| H | -1.584120 | 3.390456 | 1.712144 |
| C | -3.464120 | 2.436154 | 1.193747 |
| C | -1.775434 | 3.319055 | -0.446411 |
| H | -5.048377 | 1.249040 | 0.304688 |
| C | -3.782743 | 2.046643 | -1.267623 |
| H | -2.137149 | 2.733859 | -2.503416 |
| H | -4.031851 | 3.373884 | 1.143645 |
| H | -3.612830 | 2.022970 | 2.199984 |
| H | -0.714189 | 3.535163 | -0.615580 |
| H | -2.320126 | 4.269019 | -0.522340 |
| H | -4.160105 | 1.352663 | -2.030005 |
| H | -4.358111 | 2.975974 | -1.365412 |
| C | 3.020908 | 1.810569 | 0.124973 |
| C | 3.817825 | 1.238750 | 1.105644 |
| C | 4.444967 | 0.010406 | 0.843596 |
| C | 4.301976 | -0.609529 | -0.393734 |
| C | 3.532742 | 0.000257 | -1.414916 |
| C | 2.852228 | 1.215142 | -1.140392 |
| H | 3.578397 | -0.376493 | -2.433364 |
| H | 2.341969 | 1.759106 | -1.926082 |
| H | 5.051622 | -0.451683 | 1.615871 |
| H | 4.813913 | -1.543637 | -0.599810 |
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| Cl | 2.197436 | 3.330530 | 0.453278 |



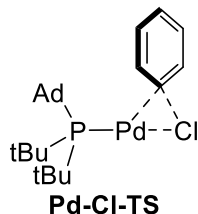
Pd-H-TS

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Pd-H-TS

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| Pd | -1.0993756209 | -0.2935143054 | -0.1158158061 |
| P | 1.1627196404 | -0.9600547194 | 0.0329523457 |
| C | 1.2924697740 | -1.8262967119 | 1.7369335329 |
| C | 1.6061333938 | -2.2165977674 | -1.3369710510 |
| C | 2.4985062415 | -2.7434330229 | 1.9371206703 |
| C | 1.2819657009 | -0.7745127139 | 2.8521790715 |
| C | -0.0106713798 | -2.6218684569 | 1.9197521256 |
| C | 1.0497510162 | -1.6720690517 | -2.6626222576 |
| C | 3.0961549188 | -2.5287630361 | -1.4844559654 |
| C | 0.8442785651 | -3.5214553760 | -1.0811123098 |
| C | 2.3714516725 | 0.5072327217 | -0.0249565801 |
| C | 2.5368980959 | 0.9781213713 | -1.4844032759 |
| C | 3.7681666195 | 0.2469223553 | 0.5643546249 |
| C | 1.7072348918 | 1.6811408117 | 0.7328594275 |
| C | 3.4023681234 | 2.2405598315 | -1.5642420726 |
| C | 4.6248116602 | 1.5175771520 | 0.4864785463 |
| C | 2.5779347377 | 2.9391499099 | 0.6688618773 |
| C | 4.7826424637 | 1.9435396829 | -0.9737690767 |
| C | 2.7415115537 | 3.3755377262 | -0.7851692340 |
| C | 3.9508161924 | 2.6413138929 | 1.2769338607 |
| H | 2.4731116095 | -3.1602190176 | 2.9580403922 |
| H | 2.5024262183 | -3.5923183924 | 1.2419890388 |
| H | 3.4505437522 | -2.2080907077 | 1.8235894165 |
| H | 0.4273241279 | -0.0880568856 | 2.7566349528 |
| H | 1.1808658988 | -1.2958193224 | 3.8181395135 |
| H | 2.2037435274 | -0.1823087170 | 2.8980996444 |
| H | -0.0406186197 | -3.0353439176 | 2.9415915852 |
| H | -0.8977767118 | -1.9704572025 | 1.8128664940 |
| H | -0.1230684880 | -3.4565736508 | 1.2212972887 |
| H | 1.5482008815 | -0.7595859369 | -3.0037012276 |
| H | 1.1871104232 | -2.4386101371 | -3.4431747118 |
| H | -0.0247455878 | -1.4530998554 | -2.5738604755 |
| H | 3.6803212069 | -1.6508018483 | -1.7897931143 |
| H | 3.5377055027 | -2.9245844836 | -0.5606143024 |
| H | 3.2289565662 | -3.2931137154 | -2.2683056598 |
| H | 1.2195978420 | -4.0821902104 | -0.2159797496 |
| H | -0.2330738775 | -3.3390379100 | -0.9488955592 |
| H | 0.9624608713 | -4.1704220868 | -1.9638731143 |
| H | 3.0168075684 | 0.1980532945 | -2.0907277127 |
| H | 1.5423764205 | 1.1708436298 | -1.9193852937 |
| H | 4.2688530610 | -0.5701786798 | 0.0238568715 |
| H | 3.6926108285 | -0.0673086547 | 1.6151081826 |
| H | 0.7157359406 | 1.8724487218 | 0.2904028573 |
| H | 1.5342295455 | 1.4250797364 | 1.7837354725 |

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|----|---------------|---------------|---------------|
| H | 3.5045210552 | 2.5242649943 | -2.6247827706 |
| H | 5.6154842854 | 1.3009749249 | 0.9196400013 |
| H | 2.0811245582 | 3.7370129329 | 1.2450635416 |
| H | 5.4264309120 | 2.8364921603 | -1.0426723424 |
| H | 5.2802088670 | 1.1449663728 | -1.5504746725 |
| H | 1.7578248690 | 3.6147059486 | -1.2221381549 |
| H | 3.3546651392 | 4.2905314144 | -0.8479691367 |
| H | 3.8421472303 | 2.3483770619 | 2.3353745237 |
| H | 4.5805390966 | 3.5468097879 | 1.2596387825 |
| C | -3.0066083046 | 0.2909624138 | -0.2269963021 |
| C | -3.9538740116 | -0.4598634454 | -0.9442907437 |
| C | -3.4882862731 | 1.3189333410 | 0.6019650746 |
| C | -5.3235050040 | -0.2419920516 | -0.7984070419 |
| C | -4.8537710563 | 1.5524136799 | 0.7611358566 |
| C | -5.7614308484 | 0.7630837688 | 0.0598965913 |
| Cl | -7.4712590119 | 1.0479428354 | 0.2477288082 |
| H | -2.7840533921 | 1.9537369262 | 1.1468633494 |
| H | -5.2167385767 | 2.3444931300 | 1.4188853355 |
| H | -1.3815783432 | 0.7338954308 | -1.2122115707 |
| H | -3.6214802077 | -1.2427896215 | -1.6314818701 |
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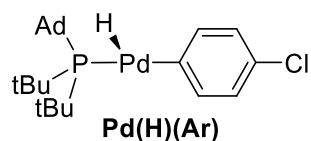


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Pd-CI-TS

| | | | |
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| Pd | -1.7581152269 | 0.7883025392 | -0.6802556199 |
| P | 0.4085517025 | 1.4312572890 | -0.2251936955 |
| C | 1.1132016587 | 2.4197956493 | -1.7115488610 |
| C | 0.4143830649 | 2.5765624331 | 1.3146291264 |
| C | 2.3485435018 | 3.2721749339 | -1.4169549401 |
| C | 1.4373955026 | 1.4459977473 | -2.8495663106 |
| C | -0.0105085879 | 3.3179320446 | -2.2519318479 |
| C | -0.5619230361 | 1.9834355256 | 2.3413548169 |
| C | 1.7811344900 | 2.8025217054 | 1.9640911198 |
| C | -0.1826053397 | 3.9353771983 | 0.9333818449 |
| C | 1.5467822864 | -0.0623854609 | 0.1156462076 |
| C | 1.2143062712 | -0.6478833968 | 1.5044717546 |
| C | 3.0578600166 | 0.2228338358 | 0.0500476314 |
| C | 1.2016145426 | -1.1695351737 | -0.9067592768 |
| C | 2.0296867055 | -1.9165626664 | 1.7793715488 |
| C | 3.8607797578 | -1.0551151033 | 0.3237705042 |
| C | 2.0223984345 | -2.4367454393 | -0.6455926935 |
| C | 3.5217812731 | -1.5861711463 | 1.7175448300 |
| C | 1.6959073957 | -2.9849595848 | 0.7416541287 |
| C | 3.5148158609 | -2.1100554737 | -0.7292132024 |
| H | 2.6863081055 | 3.7505340274 | -2.3515953116 |

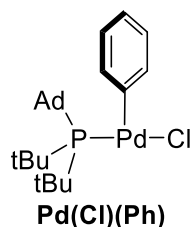
| | | | |
|----|---------------|---------------|---------------|
| H | 2.1398183732 | 4.0779357815 | -0.7019870566 |
| H | 3.1877914157 | 2.6819902344 | -1.0278570714 |
| H | 0.5821225185 | 0.7888785220 | -3.0683727404 |
| H | 1.6501379959 | 2.0319872948 | -3.7585535629 |
| H | 2.3188799514 | 0.8244840160 | -2.6493254308 |
| H | 0.3387572063 | 3.8005929831 | -3.1800276211 |
| H | -0.9068466064 | 2.7231006211 | -2.4896317583 |
| H | -0.3090597771 | 4.1109863182 | -1.5593217906 |
| H | -0.2805849566 | 0.9884358259 | 2.6991223833 |
| H | -0.6095438543 | 2.6567543291 | 3.2136631645 |
| H | -1.5687975742 | 1.9052237539 | 1.9061159778 |
| H | 2.2037457387 | 1.8817163017 | 2.3853492049 |
| H | 2.5145816497 | 3.2239248678 | 1.2649288767 |
| H | 1.6693446852 | 3.5174410063 | 2.7965296512 |
| H | 0.4769213601 | 4.5358661143 | 0.2948256623 |
| H | -1.1545600446 | 3.8175136536 | 0.4309435285 |
| H | -0.3522462948 | 4.5108757615 | 1.8580607617 |
| H | 1.4417949719 | 0.0790509206 | 2.2951585870 |
| H | 0.1369427522 | -0.8742278266 | 1.5610564320 |
| H | 3.3412785142 | 0.9967892345 | 0.7778706481 |
| H | 3.3354010303 | 0.6026783844 | -0.9436372977 |
| H | 0.1253373216 | -1.3897923330 | -0.8374364532 |
| H | 1.3894348133 | -0.8328947418 | -1.9321857491 |
| H | 1.7693203276 | -2.2815199911 | 2.7869076370 |
| H | 4.9353562146 | -0.8129743284 | 0.2688189017 |
| H | 1.7611346771 | -3.1838497190 | -1.4136445694 |
| H | 4.1211908776 | -2.4852037271 | 1.9399642866 |
| H | 3.7784821621 | -0.8328800531 | 2.4824235116 |
| H | 0.6284610308 | -3.2453260715 | 0.8042274184 |
| H | 2.2726838687 | -3.9048549275 | 0.9392808667 |
| H | 3.7678276888 | -1.7359068204 | -1.7362317498 |
| H | 4.1149624844 | -3.0213619940 | -0.5661629891 |
| C | -2.0419170224 | -3.1637334471 | 0.3313610834 |
| C | -2.0831835150 | -3.0585061350 | 1.7232109852 |
| C | -2.5322690586 | -1.8711678592 | 2.3064863907 |
| C | -2.9283555569 | -0.7940796157 | 1.5205138440 |
| C | -2.8094013680 | -0.8868986724 | 0.1229505099 |
| C | -2.4200141440 | -2.0968894463 | -0.4776481981 |
| H | -1.7167632930 | -4.0955393188 | -0.1386286696 |
| H | -1.7888847395 | -3.9033578972 | 2.3489710306 |
| H | -2.5907581663 | -1.7834771493 | 3.3944373749 |
| H | -3.3112329244 | 0.1215565724 | 1.9724836763 |
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| H | -2.4099759601 | -2.1827061115 | -1.5651264112 |



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Pd(H)(Ar)

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| P | -1.1668090118 | -0.9460551265 | -0.0228253396 |
| C | -1.2780992096 | -1.8104938472 | -1.7287012077 |
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| H | -3.4285507305 | -2.2243255406 | -1.8233969390 |
| C | -1.2785676609 | -0.7607134627 | -2.8458444973 |
| H | -0.4347132782 | -0.0613098920 | -2.7493977634 |
| H | -1.1660237631 | -1.2827819559 | -3.8101530584 |
| H | -2.2089544497 | -0.1825864066 | -2.8969397033 |
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| H | 0.0787015525 | -3.0095262742 | -2.9191015264 |
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| H | 0.1705220158 | -3.4069770809 | -1.1932924471 |
| C | -1.0606661957 | -1.6600462554 | 2.6720265309 |
| H | -1.5642135585 | -0.7491738898 | 3.0097382135 |
| H | -1.2008262373 | -2.4268160671 | 3.4517705555 |
| H | 0.0136496706 | -1.4385734497 | 2.5908461502 |
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| H | -1.1933602705 | -4.0670907370 | 0.2200750624 |
| H | 0.2450969935 | -3.3149752543 | 0.9716417706 |
| H | -0.9549882737 | -4.1583294249 | 1.9703854199 |
| C | -2.3821119628 | 0.5141508594 | 0.0305528557 |
| C | -2.5550401483 | 0.9854311452 | 1.4890170950 |
| C | -3.7762159641 | 0.2449220293 | -0.5619864786 |
| C | -1.7225496794 | 1.6901546323 | -0.7281786490 |
| H | -3.0330371121 | 0.2030967049 | 2.0940558985 |
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| C | -3.9695789490 | 2.6377000993 | -1.2782683005 |
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| H | -3.8566797833 | 2.3443651140 | -2.3361476706 |
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| Pd | 1.0985541926 | -0.2982358401 | 0.1083118701 |
| C | 3.0213555659 | 0.2447656645 | 0.1825914049 |
| C | 3.9658110260 | -0.5125734934 | 0.8976284453 |
| C | 3.5127296847 | 1.2822212466 | -0.6294349336 |
| C | 5.3367931255 | -0.2856567402 | 0.7752418219 |
| C | 4.8792386396 | 1.5265247764 | -0.7661663290 |
| H | 2.8154776021 | 1.9208320473 | -1.1795699836 |
| C | 5.7813915343 | 0.7337376498 | -0.0621294178 |
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| H | 1.1393729445 | 0.7146150445 | 1.2387904183 |
| H | 3.6318817676 | -1.3092987225 | 1.5687069682 |
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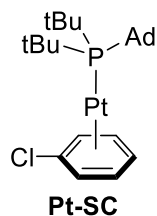


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Pd(Cl)(Ph)

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| C | 0.1060136962 | 1.9387670164 | -1.9006739471 |
| C | -0.5286645509 | 3.8288943958 | 0.8729374088 |
| H | -0.3535994740 | 4.5346249559 | 1.7019855373 |
| H | -0.2101599356 | 4.3302185570 | -0.0492270517 |
| H | -1.6108479296 | 3.6553988097 | 0.8111734212 |
| C | -0.1412540407 | 2.0170933272 | 2.5343389471 |
| H | 0.3832106602 | 1.0809855323 | 2.7764863492 |
| H | 0.1592047474 | 2.7684255906 | 3.2824474191 |
| H | -1.2208608823 | 1.8593992724 | 2.6465147298 |
| C | 1.7561668058 | 2.8396716398 | 1.2271815458 |
| H | 1.9339986016 | 3.5759999978 | 2.0284747961 |
| H | 2.3413184768 | 1.9435161762 | 1.5187659764 |
| H | 2.1816426801 | 3.2475382237 | 0.3062889631 |
| C | 0.4545840399 | 0.8352389247 | -2.9079319655 |
| H | -0.2720474722 | 0.0175029268 | -2.9421219498 |
| H | 0.5052259936 | 1.2831022948 | -3.9137958269 |
| H | 1.4413205746 | 0.4098210813 | -2.6775786003 |
| C | -1.1739730065 | 2.6565504453 | -2.3326596505 |
| H | -2.0207373818 | 1.9698846067 | -2.4548991190 |
| H | -1.4737039438 | 3.4457186313 | -1.6317330022 |
| H | -0.9994577353 | 3.1323885093 | -3.3116412374 |
| C | 1.2773189315 | 2.9255818396 | -1.9715954669 |
| H | 1.1214323418 | 3.8326280111 | -1.3764833383 |
| H | 2.2229866287 | 2.4537592030 | -1.6651450260 |
| H | 1.3951929999 | 3.2409162314 | -3.0206392484 |
| C | -1.6366344214 | 0.2795650765 | 0.0897722709 |
| C | -1.9362609398 | -0.5956844323 | -1.1460898919 |

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|----|---------------|---------------|---------------|
| C | -2.8295288092 | 1.2249666239 | 0.3248152530 |
| C | -1.5175537024 | -0.6748475825 | 1.2986486747 |
| H | -2.0552547052 | 0.0294320115 | -2.0412249115 |
| H | -1.0960163319 | -1.2828781308 | -1.3271271196 |
| C | -3.2262583922 | -1.3977186232 | -0.9496835165 |
| H | -2.9525162778 | 1.9183670803 | -0.5190347753 |
| H | -2.6609956674 | 1.8382544738 | 1.2217826008 |
| C | -4.1197557703 | 0.4136212510 | 0.5145137552 |
| H | -0.6813677498 | -1.3654666875 | 1.1361179469 |
| H | -1.3009043640 | -0.1201288563 | 2.2174057434 |
| C | -2.8115051877 | -1.4699695864 | 1.4953960631 |
| H | -3.4016890474 | -1.9948925446 | -1.8595612978 |
| C | -4.3907862213 | -0.4309051578 | -0.7319192724 |
| C | -3.0788093353 | -2.3227407195 | 0.2566275474 |
| H | -4.9527484185 | 1.1178548920 | 0.6760831957 |
| C | -3.9755260696 | -0.5058692339 | 1.7285973133 |
| H | -2.6838821004 | -2.1213252311 | 2.3755259939 |
| H | -5.3346817169 | -0.9887762533 | -0.6126074747 |
| H | -4.5144213538 | 0.2208189692 | -1.6140743266 |
| H | -2.2450546968 | -3.0260818048 | 0.0947847396 |
| H | -3.9941284897 | -2.9233738436 | 0.3921185926 |
| H | -3.7974886489 | 0.0919431324 | 2.6389742643 |
| H | -4.9113566518 | -1.0663833647 | 1.8920363869 |
| Pd | 2.0036288991 | 0.0381496415 | 0.2429361883 |
| Cl | 4.1509323838 | -0.6123481378 | 0.7707417471 |
| C | 1.4394849800 | -1.7888001933 | -0.1666721301 |
| C | 1.2726225118 | -2.6557027223 | 0.9186427473 |
| C | 1.2676341278 | -2.2679258861 | -1.4648001111 |
| C | 0.8715409664 | -3.9744946529 | 0.7026381958 |
| H | 1.4597035952 | -2.3068836974 | 1.9360224095 |
| C | 0.8705907706 | -3.5923010675 | -1.6722174207 |
| H | 1.4402377680 | -1.6238464811 | -2.3260141894 |
| C | 0.6559190761 | -4.4451867955 | -0.5924051314 |
| H | 0.7378844792 | -4.6405380545 | 1.5591048019 |
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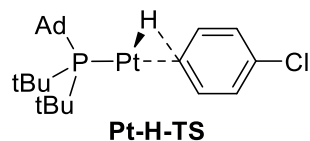
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Pt-SC

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| C | -0.4364557007 | 1.5492250554 | -2.1069394892 |
| C | -2.3286005367 | 3.4954916842 | -0.0110047577 |
| H | -2.6251884195 | 4.3367015554 | 0.6377574758 |
| H | -1.9985511114 | 3.9275900209 | -0.9647400380 |

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|----|---------------|---------------|---------------|
| H | -3.2283124915 | 2.8961434438 | -0.2018597264 |
| C | -1.7045169973 | 2.2907926675 | 2.0814122888 |
| H | -0.9456730583 | 1.6881066307 | 2.6022099791 |
| H | -1.8705995838 | 3.2071054274 | 2.6711587698 |
| H | -2.6505442344 | 1.7357817089 | 2.0688305107 |
| C | 0.0000070019 | 3.5944000954 | 0.9136531606 |
| H | -0.2916223351 | 4.4297700319 | 1.5720471333 |
| H | 0.8064409897 | 3.0264277632 | 1.4046146448 |
| H | 0.4052308619 | 4.0244096425 | -0.0076433379 |
| C | 0.4680844276 | 0.4843552604 | -2.7484404357 |
| H | 0.0145998090 | -0.5108459191 | -2.7950252744 |
| H | 0.6956329759 | 0.7966945312 | -3.7814546975 |
| H | 1.4117201228 | 0.3925801876 | -2.1882340953 |
| C | -1.7446376516 | 1.6626510793 | -2.8898867554 |
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| H | -2.4259224131 | 2.4132344328 | -2.4694372294 |
| H | -1.5179258334 | 1.9650211750 | -3.9258941158 |
| C | 0.3388352970 | 2.8651155367 | -2.2317967188 |
| H | -0.2416045738 | 3.7418807984 | -1.9194817427 |
| H | 1.2748475389 | 2.8306442432 | -1.6540115193 |
| H | 0.6058246373 | 3.0117429741 | -3.2910351319 |
| Pt | 1.3516633895 | 0.3961277880 | 0.5671785284 |
| C | -1.9337402128 | -0.2531925010 | -0.0496877180 |
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| H | -1.7497195957 | -0.9874389442 | -2.0990453433 |
| H | -0.5783568744 | -1.6831773962 | -0.9612472545 |
| C | -2.5661389443 | -2.5609151106 | -0.8954558986 |
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| H | -0.7013108664 | -1.2129972699 | 1.4482932333 |
| H | -1.9332132972 | -0.1648060811 | 2.1426461760 |
| C | -2.6994565674 | -2.0827205348 | 1.5340448937 |
| H | -2.3170245850 | -3.3142702787 | -1.6611241273 |
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| C | -2.3831768053 | -3.1585541917 | 0.4976774176 |
| H | -5.3757838690 | -0.6868181537 | -0.1551935274 |
| C | -4.1465955972 | -1.6130252198 | 1.3702075833 |
| H | -2.5530133340 | -2.4871503726 | 2.5494350688 |
| H | -4.7042218516 | -2.9490938014 | -0.9722412419 |
| H | -4.1565128831 | -1.6889849620 | -2.0921866129 |
| H | -1.3464113480 | -3.5127301046 | 0.6224318641 |
| H | -3.0451426284 | -4.0312133283 | 0.6310702194 |
| H | -4.3887063116 | -0.8547164139 | 2.1346784430 |
| H | -4.8417119867 | -2.4558380604 | 1.5241862897 |
| C | 2.7800986042 | -2.0483624167 | -0.2212085173 |
| C | 3.7179256640 | -1.5959628824 | -1.1220663319 |
| C | 4.4408251512 | -0.4166518397 | -0.8368525612 |
| C | 4.2384691092 | 0.2633790011 | 0.3473135670 |
| C | 3.3026124759 | -0.2141782719 | 1.3100282508 |

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| H | 5.1695487301 | -0.0500761367 | -1.5628653603 |
| H | 4.8234186677 | 1.1571435386 | 0.5751497473 |
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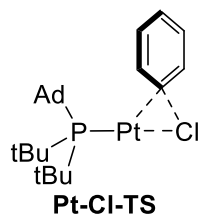


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Pt-H-TS

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| H | -2.1580946860 | -0.0387368338 | -2.9775852142 |
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| H | 0.1964193313 | -3.2979087546 | 0.8249062821 |
| H | -1.0161504448 | -4.2306819227 | 1.7300299071 |
| H | -3.1957242925 | 0.0624602743 | 1.9797189159 |
| H | -1.7442167027 | 1.0816915218 | 1.9217645235 |
| H | -4.3374130451 | -0.6309713327 | -0.2176038091 |
| H | -3.7166403903 | -0.0254015152 | -1.7562143633 |
| H | -0.8563500446 | 1.9250132975 | -0.2198868853 |
| H | -1.6060580103 | 1.5349873607 | -1.7637564363 |
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| H | -2.2461858139 | 3.7986625141 | -1.1294174256 |
| H | -5.6432981948 | 2.6787084395 | 0.9791981590 |
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| H | -2.0092974697 | 3.5559916493 | 1.3384647202 |
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| H | 5.1008871883 | 2.4174561031 | -1.3290321096 |
| H | 1.6307213903 | 0.7952501019 | 1.2668090847 |
| H | 3.5119526180 | -1.2061635959 | 1.6830577508 |
| H | 5.9441254546 | -0.8830513374 | 1.3005732836 |

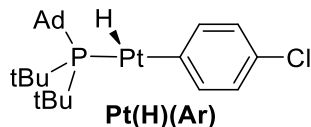


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Pt-Cl-TS

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| Pt | 1.4559018177 | -0.6972117829 | -0.3796869714 |
| Cl | 3.7355762610 | -0.0602403595 | -0.8024464983 |
| P | -0.6286766047 | -1.1835358335 | 0.1627546873 |
| C | -1.3112703649 | -2.6099928416 | -0.9304555314 |
| C | -0.6958995697 | -1.7433358175 | 1.9989211608 |
| C | -2.5734970428 | -3.2941390162 | -0.4024238504 |
| C | -1.5839734126 | -2.0652888236 | -2.3366875581 |
| C | -0.1992753487 | -3.6553368926 | -1.1041115769 |
| C | 0.2571044981 | -0.8492039988 | 2.8062277434 |
| C | -2.0853387620 | -1.7312826624 | 2.6407199874 |
| C | -0.1121912077 | -3.1562191502 | 2.1096171941 |
| C | -1.7529654827 | 0.3474991154 | -0.0518847759 |
| C | -1.4498994021 | 1.3521704065 | 1.0790934075 |
| C | -3.2643312679 | 0.0607967537 | -0.0653328200 |

| | | | |
|---|---------------|---------------|---------------|
| C | -1.3682928708 | 1.0562142799 | -1.3707240496 |
| C | -2.2530660478 | 2.6453996587 | 0.9026742691 |
| C | -4.0572658787 | 1.3622330262 | -0.2429830638 |
| C | -2.1784726685 | 2.3435256290 | -1.5593494127 |
| C | -3.7472302847 | 2.3180491899 | 0.9102750731 |
| C | -1.8798932408 | 3.3130228099 | -0.4182487056 |
| C | -3.6726129698 | 2.0144662326 | -1.5724836416 |
| C | 1.8519560708 | 3.4969249169 | -0.3985087920 |
| C | 1.8622414570 | 3.7054513280 | 0.9818326073 |
| C | 2.3665338974 | 2.7114038946 | 1.8240037651 |
| C | 2.8465487345 | 1.5138942843 | 1.3056937836 |
| C | 2.7530447899 | 1.2926901539 | -0.0762269833 |
| C | 2.3111394044 | 2.3021164699 | -0.9432230331 |
| H | -2.8968628386 | -4.0555697263 | -1.1318372968 |
| H | -2.4016288093 | -3.8154191341 | 0.5480226610 |
| H | -3.4110590930 | -2.5990706948 | -0.2622178645 |
| H | -0.7064739553 | -1.5308904038 | -2.7306192100 |
| H | -1.7880279750 | -2.9171703784 | -3.0056850055 |
| H | -2.4549377530 | -1.3998359260 | -2.3811375328 |
| H | -0.5394055975 | -4.4087378949 | -1.8343226577 |
| H | 0.7189686380 | -3.1815979266 | -1.4837341775 |
| H | 0.0546462250 | -4.1807228804 | -0.1781804763 |
| H | -0.0224485557 | 0.2091848666 | 2.8114111332 |
| H | 0.2694374866 | -1.2029620964 | 3.8510501761 |
| H | 1.2741052475 | -0.9191928000 | 2.3939065825 |
| H | -2.5027191088 | -0.7198875882 | 2.7273981935 |
| H | -2.8090357479 | -2.3517939708 | 2.0974271390 |
| H | -2.0076668130 | -2.1367593545 | 3.6634437292 |
| H | -0.7644835640 | -3.9294259765 | 1.6854919127 |
| H | 0.8738483801 | -3.2154526167 | 1.6254990912 |
| H | 0.0212785154 | -3.3928513278 | 3.1779097949 |
| H | -1.7094446340 | 0.9241428714 | 2.0557762988 |
| H | -0.3697191578 | 1.5720983136 | 1.0906228550 |
| H | -3.5776281942 | -0.4350729506 | 0.8644679209 |
| H | -3.5174792875 | -0.6196817055 | -0.8904751984 |
| H | -0.2887594414 | 1.2728201078 | -1.3477295559 |
| H | -1.5359669595 | 0.4016516898 | -2.2331568243 |
| H | -2.0131318932 | 3.3191215287 | 1.7422156443 |
| H | -5.1331433170 | 1.1195222685 | -0.2455515356 |
| H | -1.8892338758 | 2.7982850290 | -2.5215829317 |
| H | -4.3417026573 | 3.2419615177 | 0.8097800023 |
| H | -4.0319445549 | 1.8559979419 | 1.8713413525 |
| H | -0.8109770672 | 3.5748130383 | -0.4143685833 |
| H | -2.4484482596 | 4.2500402017 | -0.5485602985 |
| H | -3.9054069435 | 1.3328343493 | -2.4086150217 |
| H | -4.2649017700 | 2.9316516126 | -1.7319339548 |
| H | 2.3990878670 | 2.8725561388 | 2.9042587494 |
| H | 3.2595354435 | 0.7397348414 | 1.9527297635 |
| H | 1.4980541522 | 4.6466038225 | 1.3983686479 |
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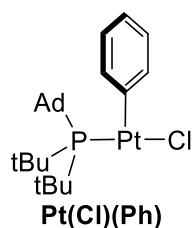


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Pt(H)(Ar)

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| P | -1.2683532894 | -0.8674242644 | -0.0118900930 |
| C | -1.2730317593 | -1.6730310378 | -1.7503878513 |
| C | -1.7243213980 | -2.1872344105 | 1.2914983577 |
| C | -2.3973193667 | -2.6660555257 | -2.0361970107 |
| H | -2.2884774179 | -3.0531264707 | -3.0632772391 |
| H | -2.3845369616 | -3.5307396320 | -1.3616051638 |
| H | -3.3873390980 | -2.1952019608 | -1.9656530281 |
| C | -1.2868111719 | -0.5946478372 | -2.8400492100 |
| H | -0.4849688742 | 0.1438061172 | -2.6940830001 |
| H | -1.1116367702 | -1.0858788671 | -3.8112326591 |
| H | -2.2444825206 | -0.0654746322 | -2.9131732101 |
| C | 0.0995523918 | -2.3575158558 | -1.8748806662 |
| H | 0.2235428533 | -2.7507272401 | -2.8977120015 |
| H | 0.9293232054 | -1.6290092500 | -1.7371447379 |
| H | 0.2545292135 | -3.1849559523 | -1.1761783947 |
| C | -1.2537701393 | -1.6712037010 | 2.6610981132 |
| H | -1.7976118517 | -0.7871627849 | 3.0077929149 |
| H | -1.4064382687 | -2.4688545473 | 3.4066769141 |
| H | -0.1829894286 | -1.4216593377 | 2.6349156057 |
| C | -3.2069359495 | -2.5578155398 | 1.3524560804 |
| H | -3.8370281076 | -1.7135957378 | 1.6622536804 |
| H | -3.5887874150 | -2.9322979463 | 0.3935585247 |
| H | -3.3477059603 | -3.3571420092 | 2.0989222197 |
| C | -0.8957770516 | -3.4502704509 | 1.0305383524 |
| H | -1.1893921664 | -3.9866074716 | 0.1199286359 |
| H | 0.1781467205 | -3.2162878158 | 0.9779920304 |
| H | -1.0427887793 | -4.1417758341 | 1.8758376099 |
| C | -2.5229703007 | 0.5559594154 | 0.0401168274 |
| C | -2.7621928370 | 0.9777475523 | 1.5044128234 |
| C | -3.8876078102 | 0.2601609436 | -0.6075740808 |
| C | -1.8762888800 | 1.7717121357 | -0.6649742592 |
| H | -3.2390777483 | 0.1638209250 | 2.0669705739 |
| H | -1.7954929711 | 1.1915829929 | 1.9888809144 |
| C | -3.6730030309 | 2.2075413006 | 1.5833964872 |
| H | -4.3782588429 | -0.5873946198 | -0.1062303937 |
| H | -3.7619687611 | -0.0246037195 | -1.6619854311 |
| C | -4.7920906608 | 1.4973227473 | -0.5293154379 |
| H | -0.9060546854 | 1.9868737921 | -0.1898989069 |
| H | -1.6611459651 | 1.5480841214 | -1.7153918777 |
| C | -2.7941900310 | 2.9955772345 | -0.5997798790 |
| H | -3.8239582604 | 2.4593153549 | 2.6461344596 |
| C | -5.0190215579 | 1.8780970585 | 0.9346545759 |
| C | -3.0252130216 | 3.3852177349 | 0.8583309969 |
| H | -5.7576828239 | 1.2566590915 | -1.0043319363 |
| C | -4.1322965100 | 2.6652487215 | -1.2653721735 |
| H | -2.3064120359 | 3.8259980648 | -1.1360952376 |

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|----|---------------|---------------|---------------|
| H | -5.6968041368 | 2.7456058898 | 1.0017613394 |
| H | -5.5080796666 | 1.0472636427 | 1.4716532627 |
| H | -2.0668195959 | 3.6461419479 | 1.3371342294 |
| H | -3.6718920981 | 4.2765600739 | 0.9236704265 |
| H | -3.9748162060 | 2.4052502655 | -2.3261992802 |
| H | -4.7955010438 | 3.5464872278 | -1.2480478747 |
| Pt | 0.9671831585 | -0.2361770791 | 0.1578271139 |
| C | 2.9423802211 | 0.2052436082 | 0.1330333728 |
| C | 3.8849758025 | -0.5588676761 | 0.8488156996 |
| C | 3.4554880827 | 1.2262101879 | -0.6913735439 |
| C | 5.2578634729 | -0.3442906574 | 0.7335934539 |
| C | 4.8237110360 | 1.4597012569 | -0.8223915889 |
| H | 2.7672102881 | 1.8635984707 | -1.2540486166 |
| C | 5.7161883680 | 0.6664606965 | -0.1067722371 |
| H | 5.2009212786 | 2.2530083249 | -1.4707645836 |
| H | 0.8616280368 | 0.7563098660 | 1.3075167276 |
| H | 3.5418087389 | -1.3508770627 | 1.5206899899 |
| Cl | 7.4311430021 | 0.9485886307 | -0.2587484473 |
| H | 5.9722583947 | -0.9514789101 | 1.2930470944 |



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Pt(Cl)(Ph)

| | | | |
|---|---------------|---------------|---------------|
| P | -0.1774444224 | 1.1496359440 | -0.1650906253 |
| C | 0.0526627371 | 2.5613469682 | 1.1135573835 |
| C | -0.1294100425 | 1.9137860666 | -1.9213666992 |
| C | -0.7099254263 | 3.8536507742 | 0.8262186453 |
| H | -0.5163161212 | 4.5696744427 | 1.6420225465 |
| H | -0.3987203840 | 4.3375794024 | -0.1074238026 |
| H | -1.7949819511 | 3.6914206082 | 0.7824970945 |
| C | -0.3290370650 | 2.0670930152 | 2.5131287767 |
| H | 0.1880502844 | 1.1299506764 | 2.7653740654 |
| H | -0.0139317871 | 2.8295697296 | 3.2438061524 |
| H | -1.4091977526 | 1.9239540237 | 2.6378122829 |
| C | 1.5666130249 | 2.8338017770 | 1.1686851562 |
| H | 1.7740936967 | 3.5641225490 | 1.9684231131 |
| H | 2.1391299783 | 1.9256024316 | 1.4629538164 |
| H | 1.9883291776 | 3.2287899807 | 0.2407366102 |
| C | 0.2000538611 | 0.8006404107 | -2.9236490831 |
| H | -0.5176140793 | -0.0256521058 | -2.9268384391 |
| H | 0.2175166487 | 1.2368989216 | -3.9357319843 |
| H | 1.1967621744 | 0.3901604909 | -2.7137170724 |
| C | -1.4169238130 | 2.6268735582 | -2.3387527995 |
| H | -2.2624891572 | 1.9366192676 | -2.4493151504 |
| H | -1.7112216818 | 3.4183666623 | -1.6380033382 |
| H | -1.2550489762 | 3.0993352212 | -3.3214392055 |

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|----|---------------|---------------|---------------|
| C | 1.0418478414 | 2.8980487176 | -2.0247705485 |
| H | 0.8951664378 | 3.8167568338 | -1.4452971254 |
| H | 1.9885390037 | 2.4276088806 | -1.7207239616 |
| H | 1.1461330760 | 3.1937204220 | -3.0809224206 |
| C | -1.8453554180 | 0.2835827917 | 0.1129135383 |
| C | -2.1595867823 | -0.6152366475 | -1.1024727017 |
| C | -3.0310764712 | 1.2403178139 | 0.3402413915 |
| C | -1.7217909880 | -0.6452876083 | 1.3409484591 |
| H | -2.2839329538 | -0.0073110839 | -2.0085896198 |
| H | -1.3247295696 | -1.3104522031 | -1.2793116608 |
| C | -3.4525058779 | -1.4049960619 | -0.8779041752 |
| H | -3.1596693436 | 1.9176235868 | -0.5153671905 |
| H | -2.8498749720 | 1.8699267675 | 1.2233586352 |
| C | -4.3241406318 | 0.4406177342 | 0.5573193945 |
| H | -0.8921516726 | -1.3446213792 | 1.1858662203 |
| H | -1.4931833690 | -0.0728863214 | 2.2458780401 |
| C | -3.0182943929 | -1.4292610404 | 1.5647614302 |
| H | -3.6396366377 | -2.0198814316 | -1.7735041614 |
| C | -4.6096704215 | -0.4271488386 | -0.6698926841 |
| C | -3.3003878001 | -2.3058317440 | 0.3460078614 |
| H | -5.1516973804 | 1.1530166566 | 0.7110008337 |
| C | -4.1752412559 | -0.4548655535 | 1.7885639296 |
| H | -2.8861504561 | -2.0631216314 | 2.4569627143 |
| H | -5.5556739693 | -0.9771616988 | -0.5320890818 |
| H | -4.7367589263 | 0.2077355590 | -1.5637852130 |
| H | -2.4720625116 | -3.0171100134 | 0.1915766161 |
| H | -4.2179084665 | -2.8983252871 | 0.5013037091 |
| H | -3.9860350534 | 0.1600942505 | 2.6851550178 |
| H | -5.1127112323 | -1.0067012422 | 1.9710744291 |
| Pt | 1.7369538495 | 0.0158676164 | 0.2706359524 |
| Cl | 3.8655474210 | -0.6377099622 | 0.8871652976 |
| C | 1.1891219289 | -1.8071491236 | -0.2231134091 |
| C | 0.9568832073 | -2.7160275964 | 0.8194886416 |
| C | 1.0913488267 | -2.2554349614 | -1.5433275769 |
| C | 0.5625062957 | -4.0242109819 | 0.5402336472 |
| H | 1.0869083965 | -2.4019267467 | 1.8566729082 |
| C | 0.6993406305 | -3.5681701755 | -1.8149167012 |
| H | 1.3215564306 | -1.5886926188 | -2.3722729370 |
| C | 0.4166287055 | -4.4542155208 | -0.7781463390 |
| H | 0.3777954077 | -4.7147659518 | 1.3673282678 |
| H | 0.6217947321 | -3.8971966925 | -2.8546433314 |
| H | 0.1069724641 | -5.4791044443 | -0.9949278604 |