Supplementary Material (ESI) for Dalton Transactions

Accurate modelling of Pd(0) + PhX oxidative addition kinetics

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Electronic Supplementary Information

Computational Methodology:

All structures were optimized in the Gaussian 03 [1] package, with the B3LYP density functional [2, 3]. The standard 6-31G(d) basis set was used, but with only the five spherical harmonic components of the polarization functions, for all H, C, P and Cl atoms. [4] For Br, Pd and I, the corresponding Stuttgart relativistic ECPs [5] were used to describe the core 28, 28 and 46 electrons, respectively, together with their associated triple zeta basis [5] as implemented in Gaussian. Additional polarization functions were added, with one f function for Pd (exponent 1.1484, [6]), and one d function each for Br and I (exponent 0.45 and 0.4, respectively). This basis set combination is denoted as BS1.

Frequencies were also calculated with B3LYP/BS1, and were used to assess the nature of stationary points, to compute zero-point energies, and to derive gas-phase statistical mechanics values for the thermal and entropic corrections at the indicated temperatures. The statistical mechanics calculations use the simple rigid-rotor harmonic oscillator approximation. Computed entropies in particular are very sensitive to numerical error in the values of the lowest-frequency modes, so these were inspected visually for all species. Soft torsional modes with frequencies lower than 30 cm^{-1} were found for most species, though no values lower than 7 cm^{-1} were obtained. Tests in which frequencies were computed again after re-optimization with tighter geometry convergence criteria did not lead to material changes in frequencies, so we estimate that the numerical error in the reported free energy terms due to incomplete geometry convergence is less than 1 kcal/mol.

Solvation free energies were obtained from single point calculations on the B3LYP/BS1 geometries with the Integral Equation Formalism Polarizable Continuum Model (IEF-PCM) continuum dielectric solvation model [7], using toluene (ε=2.379, probe radius = 2.757) as the solvent.

Additional single point energy calculations used the B3LYP/BS1 optimized geometries to obtain improved energy values with a larger basis set. This comprised the same core potential for Pd, Br and I, but now with larger aug-cc-pVTZ treatment of the valence electrons [6,8-9]. For H, C, P and Cl, the 6-311+G* all-electron basis was used [10]. This combination is denoted as BS2.

Note that the computed free energies within Gaussian use standard conditions corresponding to an ideal gas at a pressure of 1 atm at the corresponding temperature. These were converted to yield free energies with a solution phase standard state of 1 mol dm^{-3}. This was performed by adding to each species' free energy as computed in Gaussian, at the relevant temperature, a free-energy correction term equal to RT ln(V_molar_gas / V_molar_solution). In this equation, R is the gas constant, T is the absolute temperature, V_molar_gas is the volume occupied by one mole of ideal gas at the temperature considered, and V_molar_solution is the volume occupied by one mole of species in a standard solution of concentration 1 mole dm^{-3}, i.e. 1 dm^3 [11].

A final correction term was based on single-point energy calculations using the dispersion–corrected B3LYP-D functional [12] as implemented in the Orca program [13] For these

calculations, the VDZ_P basis set as implemented in ORCA was used, and was found to give similar energetics (not shown here) to BS1. However, the B3LYP-D calculations were used merely to provide a correction term $\Delta E_{disp,B3LYP\text{-}D}$ = E(B3LYP-D/VDZ_P) – E(B3LYP/VDZ_P).

Computational Method References:

[1] Gaussian 03, Revision C.02, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J. Montgomery, J. A., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Wallingford CT **2004**.
[2] A.D. Becke, *Phys. Rev. A* **1988**, *38*, 3098-3100; J.C. Slater, Quantum Theory of Molecules and Solids, Vol. 4: The Self-Consistent Field for Molecules and Solids, McGraw-Hill, New York, 1974; S.H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **1980**, *58*, 1200-1211.
[3] A.D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5652.
[4] Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213-222; Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.* **1984**, *80*, 3265-3269.
[5] Bergner, A.; Dolg, M.; Kuechle, W.; Stoll, H.; Preuss, H., *Mol. Phys.* **1993**, *80*, 1431.
[6] Peterson, K. A.; Figgen, D.; Dolg, M.; Stoll, H., *J. Chem. Phys.* **2007**, *126*, 124101.
[7] B. Marten, K. Kim, C. Cortis, R.A. Friesner, R.B. Murphy, M.N. Ringnalda, D. Sitkoff, B. Honig, *J. Phys. Chem.* **1996**, *100*, 11775; D.J. Tannor, B. Marten, R. Murphy, R.A. Friesner, D. Sitkoff, A. Nicholls, M. Ringnalda, W.A. Goddard, III, B. Honig, *J. Am. Chem. Soc.* **1994**, *116*, 11875.
[8] Peterson, K. A.; Figgen, D.; Goll, E.; Stoll, H.; Dolg, M., *J. Chem. Phys.* **2003**, *119*, 11113-11123.
[9] Peterson, K. A.; Shepler, B. C.; Figgen, D.; Stoll, H., *J. Phys. Chem.* **2006**, *110*, 13877-13883.
[10] Frisch, M. J.; Pople, J. A.; Binkley, J. S. *J. Chem. Phys.*, **1984**, *80*, 3265.
[11] C. R. Cramer et al., *Faraday Discuss* **2010**, *145*, 523-556 (doi 10.1039/B921493N), see p. 537-538
[12] Grimme, S. J. *Comput. Chem.* **2004**, *25*, 1463-1473; Grimme, S. J. *Comput. Chem.* **2006**, *27*, 1787-1799.
[13] F. Neese, *ORCA, An Ab Initio, DFT, and Semiempirical Electronic Structure Package, version 2.6.35*; Universität Bonn, Germany, **2007**

Table S1: Free energies of reaction for different phenyl halides (PhX) at 70 °C in kcal mol^{-1}
$\Delta G = \Delta G\ (343K) + \Delta G_{solv}$ (B3LYP-D/BS2)

	Cl	**Br**	**I**
PdL_2 + PhX	0.0	0.0	0.0
PdL + L + PhX	26.2	26.2	26.2
AD TS	27.6	28.6	28.4
PdL(PhX) + L	19.2	20.1	19.6
OA TS	30.7	28.3	/
PdL(Ph)(X) + L	1.4	0.2	-0.9

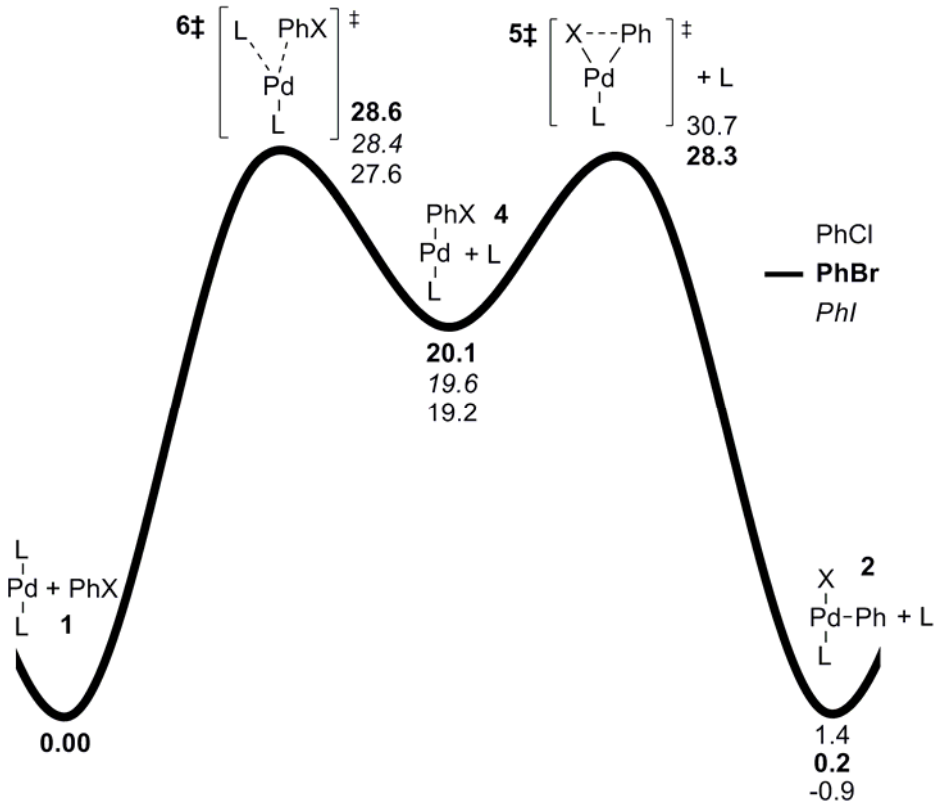

Fig. S1: Halide effects on calculated free energies of reaction for mechanism B, $\Delta G = \Delta G\ (343K) + \Delta G_{solv}$ (B3LYP-D/BS2). All energies are given in units of kcal mol^{-1} and are based on a reaction temperature of 70 ˚C for comparison. Line style and font are used to indicate identity of PhX.

Table S2: Calculated relative energies for reaction of $Pd(P^tBu_3)_2$ with PhX in kcal mol^{-1} (ΔE include ZPE corrections).

	ΔE	ΔE	ΔG (exp.T)	ΔG (exp.T) + ΔG_{solv}	ΔE	ΔG (exp.T)	ΔG (exp.T) + ΔG_{solv}
Level of Theory	B3LYP/BS1	B3LYP/BS2	B3LYP/BS2	B3LYP/BS2	B3LYP-D /BS2	B3LYP-D /BS2	B3LYP-D /BS2
Cl (T = 373K)							
PdL_2 (**1**) + PhCl	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PdL (**3**) + L + PhCl	32.8	30.7	19.4	11.3	44.8	33.5	25.4
TS [**6**‡]	25.7	27.0	39.9	39.4	16.2	29.2	28.6
PdL(PhCl) (**4**) + L	15.2	14.8	13.7	12.1	21.7	20.7	19.1
TS [**5**‡]	29.2	26.9	27.1	23.6	34.0	34.3	30.7
PdL(Ph)(Cl) (**2**) + L	6.5	3.4	4.4	-3.1	8.0	9.0	1.5
Br (T = 363K)							
PdL_2 (**1**) + PhBr	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PdL (**3**) + L + PhBr	32.8	30.7	19.7	11.6	44.8	33.8	25.7
TS [**6**‡]	25.7	27.3	39.2	39.8	16.6	28.6	29.2
PdL(PhBr) (**4**) + L	15.3	15.0	14.5	13.0	22.0	21.1	20.0
TS [**5**‡]	20.9	20.4	21.1	19.8	28.9	29.6	28.3
PdL(Ph)(Br) (**2**) + L	2.4	1.6	2.4	-4.2	5.9	6.8	0.2
I (T = 343K)							
PdL_2 (**1**) + PhI	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PdL (**3**) + L + PhI	32.8	30.7	20.2	12.1	44.8	34.3	26.2
TS [**6**‡]	25.6	27.3	39.1	39.5	16.2	28.0	28.4
PdL(PhI) (**4**) + L	15.1	14.9	14.3	12.7	21.8	21.2	19.6
TS [**5**‡]	/	/	/	/	/	/	/
PdL(Ph)(I) (**2**) + L	-1.5	-1.1	0.4	-5.2	3.2	4.7	-0.9

Table S3: Calculated "raw" relative energies for reaction of $Pd(P^tBu_3)_2$ with PhX in kcal mol^{-1}.

	$\Delta E_{B3LYP/BS1}$	$\Delta ZPE_{B3LYP/BS1}$	$\Delta E_{B3LYP/BS1} + \Delta G_{solv,B3LYP/BS1}$	$\Delta E_{B3LYP/BS2}$	$\Delta G_{B3LYP/BS1}$ (at 298 K)
Cl					
PdL_2 (**1**) + PhCl	0.0	0.0	0.0	0.0	0.0
PdL (**3**) + L + PhCl	33.5	-0.8	25.4	31.5	21.6
TS [**6**‡]	24.9	0.8	24.4	26.2	38.1
PdL(PhCl) (**4**) + L	15.7	-0.4	14.1	15.2	14.4
TS [**5**‡]	30.2	-1.0	26.6	27.9	29.4
PdL(Ph)(Cl) (**2**) + L	6.4	0.0	-1.1	3.4	7.2
Br					
PdL_2 (**1**) + PhBr	0.0	0.0	0.0	0.0	0.0
PdL (**3**) + L + PhBr	33.5	-0.8	25.4	31.5	21.6
TS [**6**‡]	25.3	0.4	25.9	26.9	37.6
PdL(PhBr) (**4**) + L	15.6	-0.3	14.1	15.3	14.9
TS [**5**‡]	21.5	-0.6	20.2	21.0	21.4
PdL(Ph)(Br) (**2**) + L	2.2	0.2	-4.3	1.4	3.1
I					
PdL_2 (**1**) + PhI	0.0	0.0	0.0	0.0	0.0
PdL (**3**) + L + PhI	33.5	-0.8	25.4	31.5	21.6
TS [**6**‡]	25.1	0.5	25.5	26.8	37.9
PdL(PhI) (**4**) + L	15.5	-0.4	13.9	15.2	14.6
TS [**5**‡]	/	/	/	/	/
PdL(Ph)(I) (**2**) + L	-2.1	0.5	-7.6	-1.6	-0.3

Experimental kinetic workings:

Experimental data values for our kinetic calculations were taken from the plots in reference 5; Barrios-Landeros, F.; Carrow, B. P.; Hartwig, J. F. *J. Am. Chem. Soc.* **2009**, *131*, 8141-8154. The data were obtained from visual inspection of the indicated Figures in reference 5 – this precludes obtaining rate constants to better than 1 significant figure, but this is enough to ensure that our estimated free energies of activation are correct to within much better than 1 kcal/mol.

$k_{obs} = ((k_B \times T) / h) \times \exp(-\Delta G_{act} / RT))$ **(Eq. 1)**
Rearrange Eq. 1 to form; $\Delta G_{act} = - RT \times \ln(k_{obs} \times (h / (k_B \times T)))$ **(Eq. 2)**

When k_{obs} = experimentally observed rate constant, $k_B = 1.38 \times 10^{-23}$ J K^{-1} Boltzmann constant, T = temperature in K, $h = 6.626 \times 10^{-34}$ J s Planck constant, ΔG_{act} = free energy of activation in kcal mol^{-1}, and R = 0.00198 kcal K^{-1} mol^{-1} is the gas constant. Note that using Eq. 2 for bimolecular reactions where k_{obs} is in s^{-1} dm^3 mol^{-1} produces a free energy of activation that implicitly contains a reference to a standard state for the translational degrees of freedom of 1 mol dm^{-3}, so is consistent with the free energies as computed in this work.

PhI
$[Pd(P^tBu_3)_2]$ at 70 °C (Fig. 3)[5]
Associative displacement is rate-limiting, therefore second order behaviour (Fig. 6) [5]:
Rate = k_2 [PhI][PdL_2]
$1 / k_{obs} \approx 700$ s for [PhI] = 1 M. Therefore $k_2 = 1/700$ s^{-1} M^{-1}.
Substituting k_2 for k in Eq. 2 above, we get $\Delta G_{act} = 24.6$ kcal mol^{-1} at 70 °C.

PhBr
$[Pd(P^tBu_2Ad)_2]$ at 90 °C, $k_{obs} \approx 2 \times 10^{-4}$ s^{-1} (Fig. 10) for [PhBr] = 1 M.[5]
Assume associative displacement is rate-limiting as for PhI, therefore same rate equation (Eq. 2), k_2 at 90 °C is 2×10^{-4} M^{-1} s^{-1}.
This is equivalent to $\Delta G_{act} = 27.4$ kcal mol^{-1} at 90 °C.
We note that in the case of bromide, a competing contribution from mechanism (i) is found (reference 5) at low PhBr concentration. However, this is not experimentally distinguishable from a mechanism involving associative displacement of L by toluene, which seems more likely based on the present calculations.

PhCl
$[Pd(P^tBu_2Cy)_2]$ at 100 °C (Fig. 8) [5]
Clear inverse first order behaviour, $(1 / k_{obs}) \approx 7000$ s^{-1} for [PhCl] = 1 M, with [L] = 0.32 M.
Rate = $k_1[PdL_2][PhCl] / [L] = k_{obs}[PdL_2]$ (**Eq. 3**)
We can rearrange Eq. 3 so that; $k_1 = k_{obs}[L] / [PhCl] = (1/7000) \times 0.32$ s^{-1}.
This corresponds to $\Delta G_{act} = 29.3$ kcal mol^{-1} at 100 °C.

Summary

PhX	**L, Expt.**	**Experimental ΔG_{act}** [kcal mol^{-1}]	**Computed ΔG_{act} barrier** [L = P^tBu_3, kcal mol^{-1}]
PhBr	P^tBu_2Ad	27.4	29.2
PhCl	P^tBu_2Cy	29.3	30.7
PhI	P^tBu_3	24.6	28.4

Cartesian Coordinates in Å for all optimised geometries (B3LYP/BS1):
$E_{B3LYP/BS1}$ / $G_{B3LYP/BS1}$ (at 298 K) in a.u
(Unless otherwise stated, no negative frequencies were determined)

PhBr.log
-245.025813 / -244.965436

C	0.0000	1.2172	-0.7878
C	0.0000	1.2078	-2.1847
C	0.0000	0.0000	-2.8849
C	0.0000	-1.2078	-2.1847
C	0.0000	-1.2172	-0.7878
C	0.0000	0.0000	-0.1076
H	0.0000	2.1527	-0.2391
H	0.0000	2.1520	-2.7224
H	0.0000	0.0000	-3.9711
H	0.0000	-2.1520	-2.7224
H	0.0000	-2.1527	-0.2391
Br	0.0000	0.0000	1.8148

PhCl.log
-691.836754 / -691.774626

C	0.0000	1.2163	-0.1782
C	0.0000	1.2077	-1.5747
C	0.0000	0.0000	-2.2754
C	0.0000	-1.2077	-1.5747
C	0.0000	-1.2163	-0.1782
C	0.0000	0.0000	0.5040
H	0.0000	2.1500	0.3739
H	0.0000	2.1517	-2.1126
H	0.0000	0.0000	-3.3616
H	0.0000	-2.1517	-2.1126
H	0.0000	-2.1500	0.3739
Cl	0.0000	0.0000	2.2649

PhI.log
-243.057049 / -242.997907

C	0.0000	1.2165	-1.2593
C	0.0000	1.2073	-2.6568
C	0.0000	0.0000	-3.3573
C	0.0000	-1.2073	-2.6568
C	0.0000	-1.2165	-1.2593
C	0.0000	0.0000	-0.5763
H	0.0000	2.1562	-0.7178
H	0.0000	2.1519	-3.1941
H	0.0000	0.0000	-4.4435
H	0.0000	-2.1519	-3.1941
H	0.0000	-2.1562	-0.7178
I	0.0000	0.0000	1.5634

L.log
-814.865317 / -814.533897

P	0.0000	0.0000	0.7067
C	0.0000	1.8185	0.0011
C	-1.5749	-0.9093	0.0011
C	1.5749	-0.9093	0.0011
C	2.7669	-0.4843	0.8955
H	2.5505	-0.6661	1.9538
H	3.6497	-1.0803	0.6252
H	3.0397	0.5658	0.7852
C	1.9396	-0.6718	-1.4778
H	2.1860	0.3728	-1.6867
H	1.1380	-0.9717	-2.1587
H	2.8277	-1.2670	-1.7360
C	1.4244	-2.4305	0.2229
H	2.3902	-2.9140	0.0227
H	0.6924	-2.8894	-0.4454
H	1.1488	-2.6676	1.2561
C	1.3927	2.4488	0.2229
H	1.3285	3.5270	0.0227
H	1.7358	2.3287	1.2561
H	2.1561	2.0443	-0.4454
C	-0.9641	2.6384	0.8955
H	-0.6984	2.5418	1.9538
H	-2.0098	2.3495	0.7852
H	-0.8893	3.7009	0.6252
C	-0.3880	2.0156	-1.4778
H	-0.3166	3.0824	-1.7360
H	-1.4158	1.7067	-1.6867
H	0.2725	1.4714	-2.1587
C	-2.8171	-0.0183	0.2229
H	-2.8484	0.8451	-0.4454
H	-2.8846	0.3389	1.2561
H	-3.7187	-0.6130	0.0227
C	-1.8028	-2.1541	0.8955
H	-1.8521	-1.8758	1.9538
H	-1.0298	-2.9153	0.7852
H	-2.7604	-2.6206	0.6252
C	-1.5516	-1.3439	-1.4778
H	-2.5111	-1.8154	-1.7360
H	-0.7701	-2.0795	-1.6867
H	-1.4105	-0.4997	-2.1587

PdL.log (**3**)
-942.817954 / -942.490635

Pd	2.1051	-0.0001	0.0008
P	-0.1440	-0.0001	0.0005
C	-0.8343	1.7984	-0.3315
C	-0.8348	-1.1859	-1.3902
C	-0.8367	-0.6124	1.7221
C	0.0142	0.0302	2.8433
H	1.0789	-0.1729	2.6885
H	-0.2877	-0.4061	3.8054
H	-0.1134	1.1101	2.9201
C	-2.3268	-0.3187	1.9926
H	-2.5372	0.7517	2.0595
H	-2.9885	-0.7477	1.2360
H	-2.6079	-0.7596	2.9587
C	-0.6036	-2.1343	1.8444
H	-0.8053	-2.4356	2.8807
H	-1.2653	-2.7240	1.2059
H	0.4338	-2.4000	1.6172
C	-0.6105	2.6677	0.9258
H	-0.8183	3.7141	0.6663
H	0.4254	2.6116	1.2748
H	-1.2753	2.4059	1.7520
C	0.0247	2.4473	-1.4432
H	1.0884	2.4066	-1.1861
H	-0.1019	1.9792	-2.4196
H	-0.2699	3.5011	-1.5431
C	-2.3221	1.8912	-0.7305
H	-2.5970	2.9495	-0.8363
H	-2.5302	1.4130	-1.6905
H	-2.9902	1.4565	0.0170
C	-0.6108	-0.5312	-2.7712
H	-1.2777	0.3132	-2.9594
H	0.4245	-0.1978	-2.8939
H	-0.8147	-1.2800	-3.5478
C	0.0232	-2.4740	-1.3967
H	1.0874	-2.2327	-1.4876
H	-0.1067	-3.0864	-0.5041
H	-0.2701	-3.0860	-2.2607
C	-2.3225	-1.5777	-1.2690
H	-2.5984	-2.1997	-2.1316
H	-2.5298	-2.1683	-0.3733
H	-2.9901	-0.7126	-1.2666

PdL2.log (**1**)
-1757.736672 / -1757.058889

Pd	0.0009	-0.0058	0.0070
P	2.3475	-0.0019	0.0024
C	3.0430	-0.5022	-1.7534
C	3.0430	1.7703	0.4373
C	3.0633	-1.2633	1.3095
C	2.8095	0.6620	-2.7417
H	3.0109	0.3019	-3.7597
H	1.7729	1.0134	-2.7126
H	3.4735	1.5115	-2.5662
C	4.5308	-0.9029	-1.8202
H	5.1987	-0.1143	-1.4639
H	4.7990	-1.1093	-2.8660
H	4.7460	-1.8116	-1.2521

C	2.1810	-1.6735	-2.2856
H	2.4644	-1.8766	-3.3279
H	2.3151	-2.5990	-1.7246
H	1.1172	-1.4146	-2.2572
C	2.1682	2.8134	-0.3008
H	2.4535	3.8187	0.0398
H	2.2873	2.7895	-1.3840
H	1.1078	2.6567	-0.0762
C	4.5251	2.0333	0.1031
H	4.7232	1.9992	-0.9712
H	5.2028	1.3309	0.5954
H	4.7956	3.0419	0.4460
C	2.8258	2.0431	1.9419
H	3.0283	3.1047	2.1375
H	1.7922	1.8419	2.2420
H	3.4965	1.4663	2.5827
C	4.5504	-1.1017	1.6848
H	4.8313	-1.8998	2.3863
H	5.2170	-1.1796	0.8217
H	4.7538	-0.1519	2.1862
C	2.8445	-2.7029	0.7935
H	3.0587	-3.4035	1.6118
H	1.8080	-2.8646	0.4799
H	3.5070	-2.9657	-0.0344
C	2.2064	-1.1506	2.5943
H	2.5031	-1.9496	3.2882
H	2.3320	-0.2020	3.1170
H	1.1426	-1.2680	2.3623
P	-2.3456	-0.0013	0.0008
C	-3.0535	-1.6218	-0.8292
C	-3.0533	0.0943	1.8183
C	-3.0421	1.5313	-0.9904
C	-2.1748	1.7048	-2.2614
H	-1.1119	1.7552	-2.0030
H	-2.4592	2.6431	-2.7582
H	-2.3046	0.9002	-2.9855
C	-4.5263	1.4690	-1.4035
H	-4.7297	0.6626	-2.1129
H	-5.1984	1.3472	-0.5505
H	-4.7990	2.4095	-1.9026
C	-2.8197	2.8147	-0.1602
H	-3.0234	3.6841	-0.7997
H	-3.4863	2.8889	0.7020
H	-1.7844	2.8942	0.1876
C	-2.8338	-1.5491	-2.3568
H	-3.0417	-2.5382	-2.7866
H	-1.7989	-1.2911	-2.6041
H	-3.5000	-0.8393	-2.8522
C	-2.1914	-2.8130	-0.3432
H	-1.1281	-2.6222	-0.5232
H	-2.3160	-3.0320	0.7177
H	-2.4847	-3.7130	-0.9016
C	-4.5400	-1.9411	-0.5692
H	-4.8155	-2.8436	-1.1329
H	-4.7458	-2.1494	0.4838
H	-5.2084	-1.1393	-0.8933
C	-2.8373	-1.2670	2.5169
H	-3.5051	-2.0486	2.1475
H	-1.8031	-1.6118	2.4155
H	-3.0446	-1.1469	3.5888
C	-2.1876	1.1055	2.6103
H	-1.1248	0.8521	2.5320
H	-2.3106	2.1360	2.2758
H	-2.4794	1.0667	3.6692
C	-4.5379	0.4849	1.9628
H	-4.8161	0.4464	3.0255
H	-4.7392	1.5027	1.6186
H	-5.2074	-0.1925	1.4272

PdL(Ph)(Br).log ($\mathbf{2}_{Br}$)

-1187.893618 / -1187.485466

Pd	0.7632	-0.7372	0.0002
Br	2.7126	-2.2074	0.0645
P	-1.4467	0.1218	-0.0187
C	-2.3408	-1.2674	-1.0518
C	-2.1374	0.0808	1.8029
C	-1.8332	1.8545	-0.8052
C	3.5132	3.1780	-0.0330
C	2.9199	2.7669	1.1607
C	2.0923	1.6368	1.1935
C	1.8503	0.9211	0.0181
C	2.4658	1.3111	-1.1776
C	3.2878	2.4435	-1.1987
H	4.1571	4.0530	-0.0523
H	3.1036	3.3163	2.0812
H	1.6602	1.3234	2.1369
H	2.3270	0.7320	-2.0850
H	3.7632	2.7369	-2.1316
C	-1.6626	-2.6174	-0.7041
H	-2.0991	-3.4028	-1.3354
H	-0.5854	-2.6058	-0.9291
H	-1.7927	-2.9240	0.3328
C	-2.0862	-1.0488	-2.5600
H	-2.4360	-1.9389	-3.0985
H	-2.6315	-0.1941	-2.9657
H	-1.0213	-0.9284	-2.7825
C	-0.9653	2.0376	-2.0723
H	-1.1622	3.0392	-2.4771
H	0.0996	1.9756	-1.8425
H	-1.1906	1.3206	-2.8613
C	-1.4079	2.9771	0.1690
H	-1.4915	3.9346	-0.3611
H	-2.0475	3.0452	1.0518
H	-0.3677	2.8709	0.4894
C	-3.3139	2.0647	-1.1862
H	-3.9963	1.9431	-0.3423
H	-3.6373	1.3960	-1.9875
H	-3.4333	3.0909	-1.5580
C	-3.8617	-1.3917	-0.8285
H	-4.1176	-1.6760	0.1946
H	-4.2497	-2.1804	-1.4871
H	-4.3996	-0.4719	-1.0716
C	-1.1248	0.8095	2.7166
H	-1.5093	0.7937	3.7449
H	-0.1621	0.2913	2.7112
H	-0.9550	1.8512	2.4445
C	-2.1811	-1.3739	2.3235
H	-2.4065	-1.3434	3.3973
H	-2.9558	-1.9824	1.8523
H	-1.2154	-1.8776	2.2108
C	-3.5337	0.7098	1.9901
H	-4.2973	0.2495	1.3581
H	-3.8443	0.5667	3.0335
H	-3.5372	1.7860	1.8016

PdL(Ph)(Cl).log ($\mathbf{2}_{Cl}$)

-1634.697863 / -1634.288108

Pd	0.7217	-1.1364	0.0434
P	-1.1842	0.2417	-0.0220
C	-2.3831	-0.9183	-1.0303
C	-1.8839	0.4297	1.7876
C	-1.1290	1.9900	-0.8658
C	4.3891	1.9307	-0.0497
C	3.6981	1.7285	1.1450
C	2.6025	0.8564	1.1958
C	2.1909	0.1926	0.0375
C	2.8979	0.3689	-1.1580
C	3.9892	1.2441	-1.1975
H	5.2404	2.6052	-0.0828
H	4.0115	2.2397	2.0524
H	2.0948	0.6977	2.1400
H	2.6190	-0.1828	-2.0501
H	4.5330	1.3733	-2.1303
C	-2.0541	-2.3820	-0.6391
H	-2.6730	-3.0564	-1.2460
H	-1.0087	-2.6430	-0.8626
H	-2.2500	-2.6140	0.4069
C	-2.0721	-0.8068	-2.5396
H	-2.6196	-1.6014	-3.0624
H	-2.3951	0.1430	-2.9709
H	-1.0076	-0.9477	-2.7516
C	-0.2312	1.9245	-2.1240
H	-0.1942	2.9295	-2.5649
H	0.7907	1.6333	-1.8757
H	-0.6060	1.2482	-2.8918
C	-0.4551	3.0034	0.0870
H	-0.2932	3.9364	-0.4679
H	-1.0732	3.2499	0.9529
H	0.5220	2.6550	0.4333
C	-2.5125	2.5388	-1.2740
H	-3.2101	2.6067	-0.4367
H	-2.9813	1.9455	-2.0631
H	-2.3797	3.5533	-1.6725
C	-3.8913	-0.6684	-0.8275
H	-4.2219	-0.8699	0.1941
H	-4.4505	-1.3485	-1.4842
H	-4.1892	0.3505	-1.0873

C	-0.7407	0.9289	2.7023
H	-1.1356	1.0416	3.7207
H	0.0724	0.1990	2.7389
H	-0.3241	1.8902	2.4026
C	-2.2792	-0.9554	2.3487
H	-2.5011	-0.8384	3.4171
H	-3.1729	-1.3728	1.8810
H	-1.4633	-1.6810	2.2663
C	-3.0945	1.3760	1.9289
H	-3.9333	1.0938	1.2877
H	-3.4501	1.3361	2.9672
H	-2.8390	2.4176	1.7207
Cl	2.1653	-2.9429	0.1347

PdL(Ph)(I).log (**2**$_{I}$)
-1185.931690 / -1185.523380

Pd	0.6650	-0.4186	-0.0278
P	-1.6968	-0.0820	-0.0141
C	-2.2611	-1.6276	-1.0613
C	-2.3323	-0.3044	1.8128
C	-2.4817	1.5256	-0.7699
C	2.3973	4.0454	-0.0197
C	1.9551	3.4769	1.1751
C	1.4373	2.1752	1.1966
C	1.3508	1.4442	0.0087
C	1.8182	1.9984	-1.1891
C	2.3322	3.3001	-1.1984
H	2.8020	5.0537	-0.0301
H	2.0189	4.0373	2.1050
H	1.1205	1.7455	2.1400
H	1.8020	1.4213	-2.1082
H	2.6950	3.7208	-2.1332
C	-1.2880	-2.7896	-0.7383
H	-1.5102	-3.6323	-1.4064
H	-0.2403	-2.5138	-0.9317
H	-1.3616	-3.1576	0.2843
C	-2.0763	-1.3312	-2.5662
H	-2.2215	-2.2672	-3.1206
H	-2.8039	-0.6142	-2.9517
H	-1.0681	-0.9698	-2.7927
C	-1.6915	1.9238	-2.0385
H	-2.1060	2.8684	-2.4152
H	-0.6354	2.0882	-1.8193
H	-1.7672	1.1942	-2.8445
C	-2.3206	2.7006	0.2218
H	-2.6451	3.6185	-0.2848
H	-2.9395	2.5935	1.1153
H	-1.2794	2.8454	0.5240
C	-3.9740	1.3911	-1.1401
H	-4.6031	1.1120	-0.2921
H	-4.1408	0.6686	-1.9429
H	-4.3296	2.3634	-1.5060
C	-3.7095	-2.1018	-0.8312
H	-3.8850	-2.4420	0.1916
H	-3.9083	-2.9560	-1.4923
H	-4.4477	-1.3307	-1.0655
C	-1.5056	0.6272	2.7298
H	-1.8776	0.5222	3.7576
H	-0.4515	0.3366	2.7245
H	-1.5701	1.6814	2.4620
C	-2.0307	-1.7374	2.3082
H	-2.2328	-1.7740	3.3865
H	-2.6590	-2.4980	1.8405
H	-0.9791	-2.0084	2.1678
C	-3.8345	-0.0237	2.0235
H	-4.4750	-0.6322	1.3804
H	-4.0928	-0.2648	3.0632
H	-4.0925	1.0264	1.8678
I	3.0573	-1.5001	0.0391

PdL(PhBr).log (**4**$_{Br}$)
-1187.872338 / -1187.466717

Pd	-0.0956	-0.9781	-0.2440
Br	-4.8996	1.1575	0.0262
P	1.9097	0.1920	0.0273
C	1.8006	1.4384	1.5235
C	3.3779	-1.0464	0.3700
C	2.3326	1.2097	-1.5842
C	-1.8200	-2.4206	-0.0622
C	-2.5014	-2.0769	1.1323
C	-3.4124	-1.0284	1.1584
C	-3.6342	-0.2896	-0.0152
C	-2.9656	-0.5724	-1.1959
C	-2.0521	-1.6549	-1.2311
H	-1.2712	-3.3575	-0.1159
H	-2.3361	-2.6664	2.0299
H	-3.9473	-0.7817	2.0689
H	-3.1575	0.0042	-2.0941
H	-1.6723	-1.9871	-2.1937
C	1.8364	0.6482	2.8504
H	1.5764	1.3325	3.6689
H	1.1038	-0.1656	2.8552
H	2.8223	0.2369	3.0785
C	2.8865	2.5314	1.5778
H	3.8987	2.1209	1.6176
H	2.7424	3.1327	2.4861
H	2.8320	3.2182	0.7297
C	0.4060	2.1100	1.4803
H	0.2861	2.7292	2.3800
H	0.2620	2.7596	0.6166
H	-0.3898	1.3579	1.4713
C	2.8715	-2.1228	1.3611
H	3.6400	-2.9020	1.4596
H	2.6731	-1.7325	2.3594
H	1.9513	-2.5897	0.9934
C	4.6779	-0.4280	0.9241
H	4.5437	0.0078	1.9177
H	5.0928	0.3427	0.2697
H	5.4361	-1.2174	1.0208
C	3.7117	-1.8066	-0.9320
H	4.3927	-2.6331	-0.6894
H	2.8141	-2.2383	-1.3870
H	4.2166	-1.1836	-1.6734
C	3.7851	1.7130	-1.7097
H	3.8775	2.3084	-2.6286
H	4.0864	2.3537	-0.8770
H	4.5064	0.8953	-1.7876
C	1.3813	2.4226	-1.6845
H	1.4927	2.8703	-2.6810
H	0.3343	2.1233	-1.5709
H	1.6037	3.2059	-0.9565
C	2.0002	0.3241	-2.8100
H	2.1212	0.9257	-3.7214
H	2.6484	-0.5471	-2.9056
H	0.9649	-0.0301	-2.7645

PdL(PhCl).log (**4**$_{Cl}$)
-1634.683164 / -1634.276674

Pd	-0.5819	-0.8744	-0.2561
P	1.5081	0.1237	0.0242
C	1.4587	1.4041	1.4974
C	2.8781	-1.2073	0.4194
C	2.0335	1.0782	-1.5954
C	-2.4831	-2.0753	-0.0606
C	-3.1008	-1.6418	1.1394
C	-3.8634	-0.4816	1.1700
C	-3.9983	0.2789	-0.0031
C	-3.3846	-0.0948	-1.1888
C	-2.6239	-1.2880	-1.2297
H	-2.0627	-3.0764	-0.1168
H	-3.0054	-2.2463	2.0372
H	-4.3543	-0.1605	2.0825
H	-3.5115	0.5032	-2.0850
H	-2.2988	-1.6694	-2.1940
C	1.4070	0.6374	2.8377
H	1.1847	1.3540	3.6396
H	0.6139	-0.1176	2.8408
H	2.3528	0.1545	3.0937
C	2.6203	2.4166	1.5592
H	3.5991	1.9359	1.6361
H	2.4965	3.0476	2.4503
H	2.6382	3.0865	0.6959
C	0.1192	2.1770	1.4108
H	0.0213	2.8107	2.3030
H	0.0492	2.8290	0.5397
H	-0.7307	1.4869	1.3827
C	2.2715	-2.2328	1.4086
H	2.9882	-3.0536	1.5500
H	2.0575	-1.8136	2.3920
H	1.3401	-2.6514	1.0118
C	4.2018	-0.6692	0.9985
H	4.0705	-0.1971	1.9754
H	4.6882	0.0516	0.3364
H	4.8984	-1.5073	1.1381
C	3.1941	-2.0097	-0.8622
H	3.8074	-2.8783	-0.5875

H	2.2818	-2.3855	-1.3371
H	3.7638	-1.4379	-1.5983
C	3.5207	1.4721	-1.7001
H	3.6747	2.0431	-2.6262
H	3.8517	2.1022	-0.8709
H	4.1802	0.6020	-1.7488
C	1.1763	2.3553	-1.7322
H	1.3399	2.7787	-2.7322
H	0.1078	2.1370	-1.6352
H	1.4430	3.1299	-1.0101
C	1.6601	0.1956	-2.8114
H	1.8357	0.7711	-3.7309
H	2.2499	-0.7186	-2.8807
H	0.6025	-0.0869	-2.7768
Cl	-4.9737	1.7443	0.0410

PdL(PhI).log (**4**$_{I}$)
-1185.903755 / -1185.499673

Pd	0.3493	-1.0501	-0.2680
P	2.2781	0.2393	0.0273
C	2.0877	1.4506	1.5425
C	3.8230	-0.9075	0.3555
C	2.6397	1.3068	-1.5654
C	-1.2544	-2.6321	-0.0482
C	-1.9632	-2.3346	1.1419
C	-2.9493	-1.3556	1.1604
C	-3.2220	-0.6378	-0.0166
C	-2.5303	-0.8790	-1.1938
C	-1.5408	-1.8945	-1.2227
H	-0.6349	-3.5241	-0.0941
H	-1.7575	-2.9054	2.0434
H	-3.5009	-1.1516	2.0715
H	-2.7568	-0.3277	-2.0999
H	-1.1399	-2.2059	-2.1839
C	2.1645	0.6430	2.8573
H	1.8593	1.2975	3.6844
H	1.4830	-0.2140	2.8454
H	3.1724	0.2889	3.0854
C	3.1056	2.6060	1.6217
H	4.1406	2.2561	1.6559
H	2.9236	3.1796	2.5409
H	3.0105	3.3047	0.7869
C	0.6559	2.0385	1.5018
H	0.4950	2.6359	2.4098
H	0.4787	2.6912	0.6470
H	-0.0943	1.2413	1.4761
C	3.3859	-2.0277	1.3304
H	4.2040	-2.7555	1.4206
H	3.1602	-1.6638	2.3327
H	2.4991	-2.5485	0.9537
C	5.0797	-0.2150	0.9222
H	4.9176	0.1933	1.9233
H	5.4457	0.5922	0.2825
H	5.8872	-0.9555	1.0069
C	4.2098	-1.6260	-0.9560
H	4.9449	-2.4073	-0.7215
H	3.3448	-2.1119	-1.4196
H	4.6724	-0.9599	-1.6875
C	4.0569	1.9055	-1.6760
H	4.1145	2.5172	-2.5870
H	4.3100	2.5544	-0.8336
H	4.8311	1.1384	-1.7595
C	1.6142	2.4596	-1.6536
H	1.6996	2.9249	-2.6445
H	0.5874	2.0953	-1.5458
H	1.7866	3.2470	-0.9161
C	2.3702	0.4207	-2.8061
H	2.4591	1.0419	-3.7080
H	3.0717	-0.4072	-2.9097
H	1.3590	0.0018	-2.7735
I	-4.7474	0.8628	0.0163

ADTS_Br.log (**6**$_{Br}^{‡}$)
-2002.722145 / -2001.964402
v = –61.4 cm^{-1}

Pd	0.4097	-0.1604	0.3171
P	2.4631	-1.133	-0.0387
C	2.3914	-3.0775	-0.2887
C	3.3285	-0.3814	-1.6287
C	3.6551	-0.8011	1.4816
C	3.4546	0.6621	1.9358
C	3.2008	-1.6726	2.6731
C	5.1609	-1.0403	1.2486
C	4.5317	-1.1635	-2.1953
C	2.2513	-0.2484	-2.7317
C	3.793	1.0606	-1.3278
C	3.7165	-3.8541	-0.1427
C	1.8037	-3.3817	-1.6837
C	1.3745	-3.6482	0.7269
H	3.8265	1.3926	1.2174
H	4.0033	0.818	2.8758
H	2.3975	0.8753	2.112
H	2.1259	-1.5711	2.8577
H	3.437	-2.731	2.5425
H	3.7277	-1.3351	3.5759
H	5.5831	-0.3533	0.511
H	5.39	-2.0606	0.9332
H	5.6983	-0.864	2.1913
H	4.255	-2.1522	-2.5694
H	5.3381	-1.2901	-1.4681
H	4.9475	-0.6062	-3.0466
H	2.6936	0.2593	-3.6003
H	1.8627	-1.2076	-3.0758
H	1.407	0.351	-2.376
H	4.0682	1.5436	-2.2749
H	2.9967	1.6572	-0.8735
H	4.674	1.0981	-0.683
H	3.5344	-4.9142	-0.3701
H	4.4939	-3.5061	-0.8271
H	4.1156	-3.8138	0.8741
H	1.557	-4.4508	-1.7372
H	2.5017	-3.173	-2.4973
H	0.8831	-2.8184	-1.8621
H	0.4122	-3.1361	0.6448
H	1.2207	-4.7156	0.5141
H	1.7063	-3.5669	1.7624
C	0.5312	3.4183	0.3423
C	-0.3568	2.3778	0.6397
C	-0.4766	1.9597	1.9746
C	0.2912	2.5626	2.9773
C	1.1762	3.59	2.6524
C	1.3026	4.0267	1.328
Br	0.6631	4.0441	-1.4695
H	-1.0043	1.9667	-0.1284
H	-1.2008	1.1903	2.2236
H	0.1917	2.2332	4.0076
H	1.7698	4.0673	3.4273
H	1.9814	4.834	1.0745
P	-2.9994	-0.5512	0.015
C	-2.9901	-1.4403	-1.7213
C	-3.5672	-1.8529	1.3546
C	-4.3741	0.8421	-0.0614
C	-4.3543	-1.7013	-2.3906
C	-2.1148	-0.5721	-2.6587
C	-2.2504	-2.7893	-1.6006
C	-2.3268	-2.7066	1.7135
C	-3.9513	-1.1183	2.6584
C	-4.7292	-2.7936	0.975
C	-4.1654	1.6946	-1.3333
C	-5.8439	0.3752	-0.026
C	-4.1391	1.8127	1.1223
H	-4.1925	-2.2379	-3.3363
H	-4.8887	-0.7803	-2.6359
H	-5.0116	-2.3209	-1.7746
H	-1.1144	-0.427	-2.2339
H	-2.5419	0.41	-2.8669
H	-2.0022	-1.0893	-3.622
H	-2.8272	-3.5491	-1.068
H	-2.063	-3.1769	-2.6112
H	-1.2814	-2.6714	-1.1073
H	-2.0137	-3.3677	0.9054
H	-1.4707	-2.0766	1.9795
H	-2.5677	-3.3408	2.5782
H	-3.1722	-0.4184	2.9805
H	-4.0701	-1.8619	3.4578
H	-4.8966	-0.5759	2.5845
H	-4.4889	-3.4337	0.1224
H	-4.9474	-3.4587	1.8229
H	-5.6492	-2.2519	0.7415
H	-4.4365	1.17	-2.2513
H	-3.1329	2.0474	-1.4297
H	-4.8069	2.5839	-1.269
H	-6.0894	-0.3145	-0.837
H	-6.1038	-0.1082	0.9194
H	-6.5021	1.2498	-0.1293
H	-4.2777	1.3502	2.0997
H	-4.8599	2.6387	1.0491

H	-3.1374	2.2497	1.0937

ADTS_Cl.log (**6**$_{Cl}^{‡}$)
-2449.533717 / -2448.772747
v = –62.*7 cm*$^{-1}$

Pd	-0.4128	0.1289	-0.2359
P	-2.4692	-0.8786	0.0003
C	-2.3963	-2.8371	0.0803
C	-3.3285	-0.2680	1.6529
C	-3.6693	-0.4227	-1.4806
C	-3.4613	1.0701	-1.8225
C	-3.2353	-1.1987	-2.7439
C	-5.1743	-0.6720	-1.2515
C	-4.5274	-1.0961	2.1618
C	-2.2478	-0.2264	2.7603
C	-3.7966	1.1937	1.4803
C	-3.7232	-3.6012	-0.1031
C	-1.7824	-3.2529	1.4345
C	-1.4057	-3.3196	-1.0052
H	-3.7771	1.7454	-1.0276
H	-4.0538	1.3127	-2.7164
H	-2.4101	1.2792	-2.0365
H	-2.1589	-1.1063	-2.9236
H	-3.4960	-2.2591	-2.7067
H	-3.7554	-0.7724	-3.6125
H	-5.5878	-0.0396	-0.4619
H	-5.4034	-1.7120	-1.0077
H	-5.7198	-0.4268	-2.1739
H	-4.2448	-2.1093	2.4583
H	-5.3375	-1.1696	1.4315
H	-4.9410	-0.6080	3.0556
H	-2.6883	0.2079	3.6686
H	-1.8582	-1.2106	3.0234
H	-1.4041	0.4002	2.4540
H	-4.0867	1.5846	2.4647
H	-2.9965	1.8328	1.0965
H	-4.6682	1.2895	0.8287
H	-3.5357	-4.6765	0.0276
H	-4.4861	-3.3157	0.6245
H	-4.1430	-3.4736	-1.1040
H	-1.5400	-4.3238	1.3996
H	-2.4657	-3.1067	2.2739
H	-0.8564	-2.7087	1.6414
H	-0.4622	-2.7703	-0.9480
H	-1.1986	-4.3878	-0.8502
H	-1.7936	-3.2082	-2.0184
C	-0.6132	3.6591	0.3775
C	0.3077	2.6938	-0.0482
C	0.4618	2.4730	-1.4256
C	-0.3066	3.1932	-2.3482
C	-1.2247	4.1413	-1.8987
C	-1.3833	4.3820	-0.5289
Cl	-0.7788	3.9842	2.1005
H	0.9467	2.1941	0.6729
H	1.2176	1.7735	-1.7684
H	-0.1805	3.0165	-3.4126
H	-1.8181	4.7090	-2.6101
H	-2.0849	5.1290	-0.1723
P	2.9361	-0.3865	-0.0035
C	2.9360	-1.7332	1.4070
C	3.4882	-1.2559	-1.6620
C	4.3197	0.9194	0.4610
C	4.3023	-2.1822	1.9633
C	2.0710	-1.1639	2.5582
C	2.1911	-2.9894	0.9105
C	2.2408	-1.9737	-2.2335
C	3.8610	-0.1803	-2.7066
C	4.6543	-2.2620	-1.5783
C	4.1254	1.3716	1.9264
C	5.7866	0.4772	0.2801
C	4.0855	2.1902	-0.3923
H	4.1410	-2.9642	2.7188
H	4.8484	-1.3739	2.4555
H	4.9498	-2.6069	1.1908
H	1.0810	-0.8708	2.1902
H	2.5180	-0.2997	3.0520
H	1.9355	-1.9416	3.3229
H	2.7656	-3.5688	0.1837
H	2.0020	-3.6481	1.7690
H	1.2235	-2.7333	0.4722
H	1.9557	-2.8572	-1.6617
H	1.3724	-1.3054	-2.2654
H	2.4565	-2.3057	-3.2587
H	3.0785	0.5791	-2.8140
H	3.9770	-0.6669	-3.6842
H	4.8048	0.3232	-2.4863
H	4.4265	-3.1181	-0.9385
H	4.8611	-2.6596	-2.5823
H	5.5776	-1.8047	-1.2136
H	4.3971	0.6039	2.6536
H	3.0964	1.6887	2.1283
H	4.7745	2.2374	2.1142
H	6.0324	-0.4231	0.8479
H	6.0396	0.2957	-0.7681
H	6.4503	1.2794	0.6335
H	4.2230	2.0288	-1.4617
H	4.8075	2.9595	-0.0857
H	3.0845	2.6019	-0.2396

ADTS_I.log (**6**$_{I}^{‡}$)
-2000.753755 / -1999.996440
v = *–63.7 cm*$^{-1}$

Pd	0.3118	-0.5013	0.4091
P	2.2484	-1.635	-0.0904
C	1.9614	-3.4971	-0.6395
C	3.1873	-0.7418	-1.5609
C	3.4767	-1.6853	1.4394
C	3.433	-0.3049	2.1327
C	2.943	-2.6905	2.4834
C	4.9471	-2.0359	1.1327
C	4.2966	-1.5481	-2.2671
C	2.1269	-0.3232	-2.607
C	3.8037	0.5771	-1.0467
C	3.1947	-4.4239	-0.6543
C	1.3322	-3.5096	-2.0492
C	0.9003	-4.111	0.3034
H	3.8489	0.4982	1.5246
H	4.0238	-0.3564	3.0587
H	2.4077	-0.0287	2.3913
H	1.8849	-2.5161	2.7066
H	3.0707	-3.7317	2.1793
H	3.5063	-2.558	3.4171
H	5.4369	-1.2775	0.5167
H	5.0629	-3.0024	0.6372
H	5.5052	-2.0862	2.0784
H	3.9115	-2.428	-2.7884
H	5.0842	-1.876	-1.584
H	4.7699	-0.9099	-3.0265
H	2.6152	0.2743	-3.3897
H	1.642	-1.1691	-3.0954
H	1.3477	0.2895	-2.1418
H	4.1369	1.1673	-1.9107
H	3.0722	1.1787	-0.4993
H	4.6783	0.4198	-0.4114
H	2.8947	-5.4088	-1.0397
H	3.998	-4.0565	-1.2973
H	3.6064	-4.5881	0.3447
H	0.9688	-4.5236	-2.2652
H	2.0442	-3.2503	-2.8357
H	0.4782	-2.8296	-2.115
H	0.0057	-3.484	0.3477
H	0.6143	-5.1009	-0.0792
H	1.2596	-4.2479	1.3238
C	0.8407	3.1793	0.8241
C	-0.1516	2.1965	0.9034
C	-0.3401	1.5242	2.1217
C	0.4548	1.8357	3.2313
C	1.4401	2.816	3.1269
C	1.6413	3.4962	1.9193
H	-0.8045	1.994	0.0618
H	-1.1499	0.8051	2.2091
H	0.2988	1.315	4.1719
H	2.0566	3.067	3.986
H	2.4026	4.2655	1.846
P	-3.0791	-0.488	-0.0135
C	-3.1534	-1.3482	-1.7621
C	-3.8026	-1.7383	1.3014
C	-4.2935	1.0501	-0.0848
C	-4.5312	-1.4487	-2.4462
C	-2.1787	-0.5704	-2.6802
C	-2.5708	-2.7724	-1.6529
C	-2.6722	-2.7369	1.65
C	-4.1079	-0.982	2.6135
C	-5.0652	-2.5299	0.9026
C	-3.977	1.8923	-1.3414
C	-5.8059	0.748	-0.0701

C	-3.9682	1.9723	1.1159
H	-4.4198	-1.9915	-3.3956
H	-4.957	-0.4721	-2.6881
H	-5.2602	-1.9967	-1.8428
H	-1.1764	-0.5312	-2.2384
H	-2.4984	0.4519	-2.8876
H	-2.1052	-1.0906	-3.6455
H	-3.2365	-3.4684	-1.1375
H	-2.4145	-3.1667	-2.6662
H	-1.6016	-2.7697	-1.1472
H	-2.4585	-3.439	0.8436
H	-1.738	-2.2182	1.8944
H	-2.9744	-3.3296	2.5249
H	-3.254	-0.3871	2.9565
H	-4.3279	-1.7174	3.3987
H	-4.9783	-0.3271	2.5368
H	-4.8959	-3.1817	0.0421
H	-5.3655	-3.1761	1.7399
H	-5.9134	-1.8802	0.6724
H	-4.291	1.413	-2.2706
H	-2.9111	2.1327	-1.4204
H	-4.5197	2.8446	-1.2712
H	-6.1182	0.0999	-0.8924
H	-6.1278	0.2856	0.8668
H	-6.3618	1.6916	-0.167
H	-4.1733	1.516	2.0843
H	-4.5891	2.876	1.0455
H	-2.9234	2.2932	1.109
I	1.1106	4.2426	-1.0125

OATS_Br.log ($\mathbf{5}_{Br}^{‡}$)
-1187.862929 / -1187.456306
v = –121.2 cm^{-1}

Pd	0.7328	-0.0319	-0.0097
Br	2.4327	-2.0792	-0.0031
P	-1.6447	0.1345	-0.0034
C	-2.4562	-1.4858	-0.7175
C	-2.2808	0.3955	1.8191
C	-2.2293	1.6476	-1.0836
C	4.3252	2.4065	-0.0050
C	3.9405	1.8234	1.2066
C	3.1752	0.6548	1.2220
C	2.7589	0.0985	-0.0047
C	3.1742	0.6549	-1.2315
C	3.9400	1.8235	-1.2164
H	4.9376	3.3038	-0.0051
H	4.2504	2.2688	2.1488
H	2.9147	0.1702	2.1570
H	2.9130	0.1705	-2.1665
H	4.2500	2.2686	-2.1586
C	-2.3024	-2.6274	0.3123
H	-2.5899	-3.5706	-0.1705
H	-1.2657	-2.7334	0.6479
H	-2.9470	-2.5058	1.1856
C	-3.9419	-1.3791	-1.1154
H	-4.5809	-1.0709	-0.2839
H	-4.2935	-2.3646	-1.4503
H	-4.1043	-0.6850	-1.9441
C	-1.6305	-1.9279	-1.9503
H	-2.0074	-2.9011	-2.2933
H	-1.7020	-1.2379	-2.7914
H	-0.5722	-2.0457	-1.6956
C	-1.4596	-0.5346	2.7455
H	-1.7322	-0.3225	3.7884
H	-1.6405	-1.5949	2.5692
H	-0.3855	-0.3542	2.6299
C	-3.7840	0.1446	2.0553
H	-4.0670	-0.8984	1.8922
H	-4.4214	0.7707	1.4258
H	-4.0254	0.3803	3.1010
C	-1.9490	1.8329	2.2792
H	-2.1388	1.9049	3.3583
H	-0.8949	2.0797	2.1142
H	-2.5676	2.5920	1.7954
C	-3.6799	2.1206	-0.8607
H	-3.8979	2.9440	-1.5547
H	-4.4148	1.3337	-1.0497
H	-3.8448	2.5035	0.1494
C	-2.0506	1.3064	-2.5799
H	-2.1994	2.2231	-3.1655
H	-1.0414	0.9393	-2.7949
H	-2.7748	0.5739	-2.9429
C	-1.2631	2.8259	-0.8101
H	-1.5032	3.6466	-1.4998
H	-1.3349	3.2209	0.2034
H	-0.2224	2.5301	-0.9836

OATS_Cl.log ($\mathbf{5}_{Cl}^{‡}$)
-1634.659988 / -1634.252782
v = –196.1 cm^{-1}

Pd	-0.7336	-1.0186	0.0107
P	1.3336	0.1143	0.0019
C	2.7345	-1.1484	-0.4984
C	1.3420	1.5826	-1.2779
C	1.7546	0.8313	1.7637
C	-4.0613	2.1330	-0.0020
C	-3.7551	1.4971	-1.2092
C	-3.1492	0.2400	-1.2211
C	-2.7993	-0.3566	0.0024
C	-3.1640	0.2368	1.2229
C	-3.7693	1.4937	1.2071
H	-4.5462	3.1048	-0.0035
H	-4.0009	1.9740	-2.1548
H	-2.9394	-0.2704	-2.1547
H	-2.9638	-0.2753	2.1577
H	-4.0258	1.9684	2.1510
C	2.6218	-1.4625	-2.0069
H	3.2794	-2.3118	-2.2340
H	1.6027	-1.7505	-2.2853
H	2.9397	-0.6334	-2.6429
C	4.1822	-0.7091	-0.1977
H	4.4496	0.2330	-0.6829
H	4.8715	-1.4772	-0.5747
H	4.3760	-0.6076	0.8733
C	2.4565	-2.4888	0.2259
H	3.1720	-3.2388	-0.1382
H	2.5694	-2.4290	1.3086
H	1.4445	-2.8501	0.0123
C	0.6019	1.1144	-2.5544
H	0.5209	1.9669	-3.2427
H	1.1158	0.3137	-3.0863
H	-0.4089	0.7706	-2.3165
C	2.7313	2.1221	-1.6760
H	3.3336	1.3794	-2.2056
H	3.3090	2.4814	-0.8208
H	2.5980	2.9720	-2.3593
C	0.5023	2.7522	-0.7179
H	0.3543	3.4869	-1.5205
H	-0.4873	2.4209	-0.3884
H	0.9920	3.2757	0.1064
C	2.8986	1.8640	1.8183
H	3.0677	2.1518	2.8651
H	3.8430	1.4717	1.4329
H	2.6614	2.7793	1.2704
C	2.0977	-0.3322	2.7199
H	2.1413	0.0617	3.7439
H	1.3299	-1.1125	2.6983
H	3.0685	-0.7871	2.5111
C	0.4690	1.4744	2.3386
H	0.6637	1.7775	3.3766
H	0.1449	2.3620	1.7951
H	-0.3599	0.7606	2.3379
Cl	-2.7377	-2.3465	0.0016