Supporting Information

for

Ligand-directed Reactivity in Dioxygen and Water Binding to *cis*-$[Pd(NHC)_2(\eta^2\text{-}O_2)]$

Taryn D. Palluccio, Xiaochen Cai, Subhojit Majumdar, Leonardo Farias-Serafim, Neil C. Tomson, Karl Wieghardt,* Catherine S. J. Cazin,* Steven P. Nolan,* Elena V. Rybak-Akimova,* Miguel Ángel Fernández-González, Manuel Temprado,* Burjor Captain* and Carl D. Hoff*

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Section A. ESR and Magnetic Studies

Electron Paramagnetic Resonance Data. X-band EPR data were recorded on a Bruker ESP 300 spectrometer and simulated with XSophe,[1] distributed by Bruker Biospin GmbH.

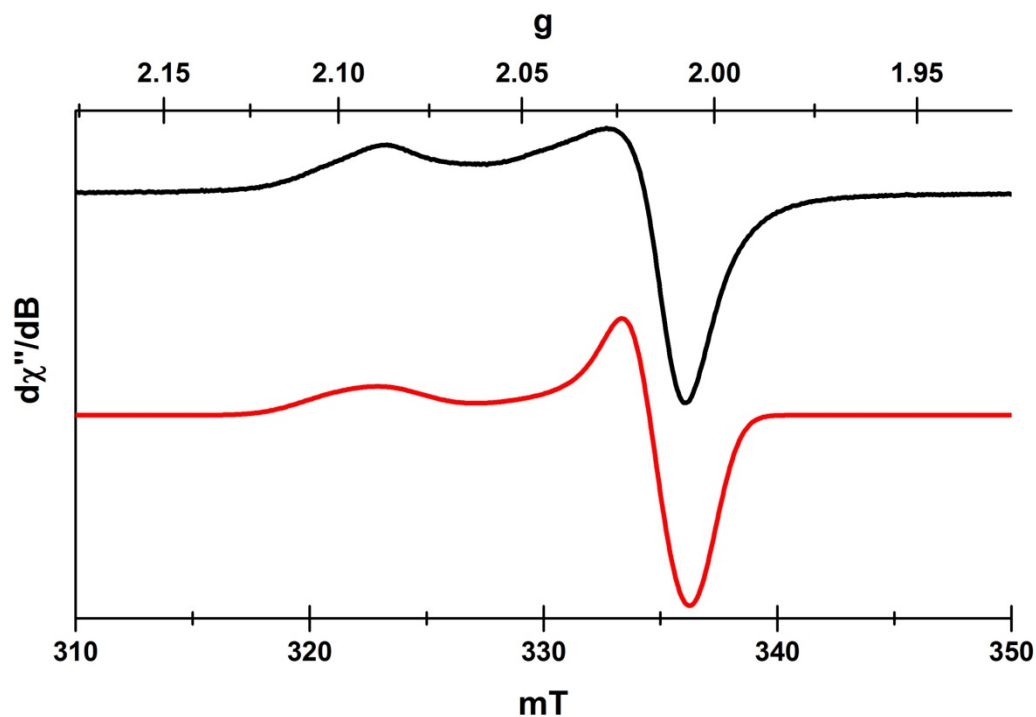**Figure S1.** Experimental EPR spectrum of solid *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] at 293 K (frequency, 9.44410 GHz; power, 0.01 mW; modulation amplitude, 15.0 G). Simulation parameters: Spin = 1; $g_x = g_y = 2.011$; $g_z = 2.095$; D = 0.00125 cm^{-1}.
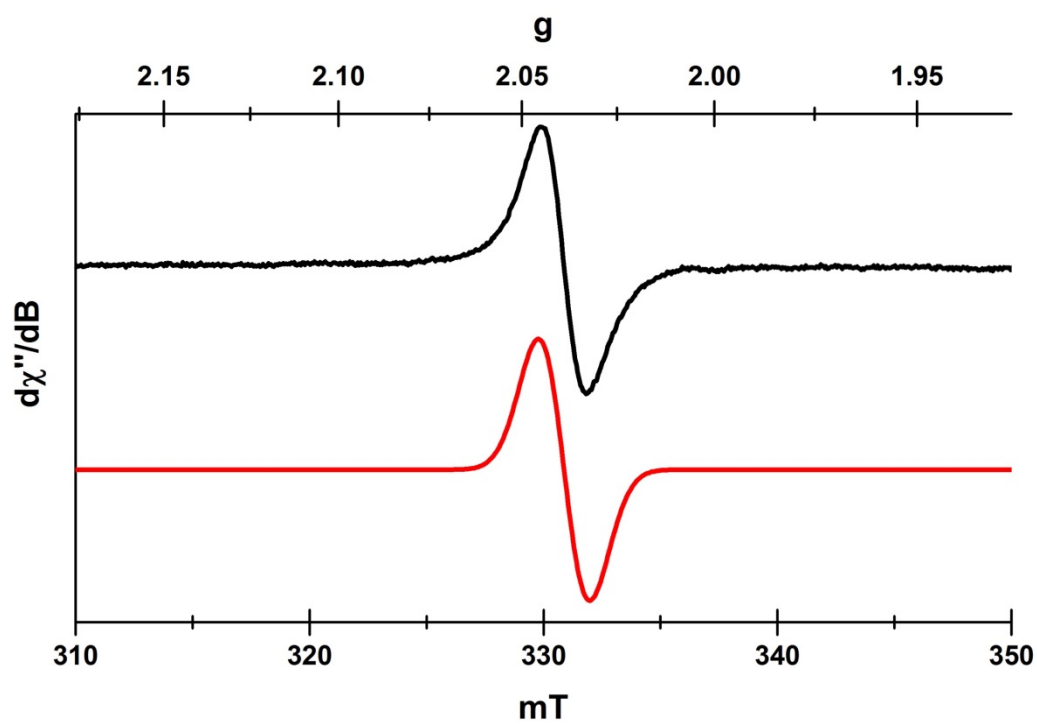
Figure S2. Experimental EPR spectrum of *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] in hexane at 293 K (frequency, 9.4417 GHz; power, 1.00 mW; modulation amplitude, 15.0 G). Simulation parameters: Spin = 1; $g_x = g_y = g_z = 2.0388$.

Magnetometry. Variable temperature (4-300 K) magnetization data were recorded in a 1 T magnetic field on a SQUID magnetometer (MPMS Quantum Design). The experimental magnetic susceptibility data were corrected for underlying diamagnetism using Pascal's constants, and an additional paramagnetic correction was applied to account for a paramagnetic impurity in the sample.
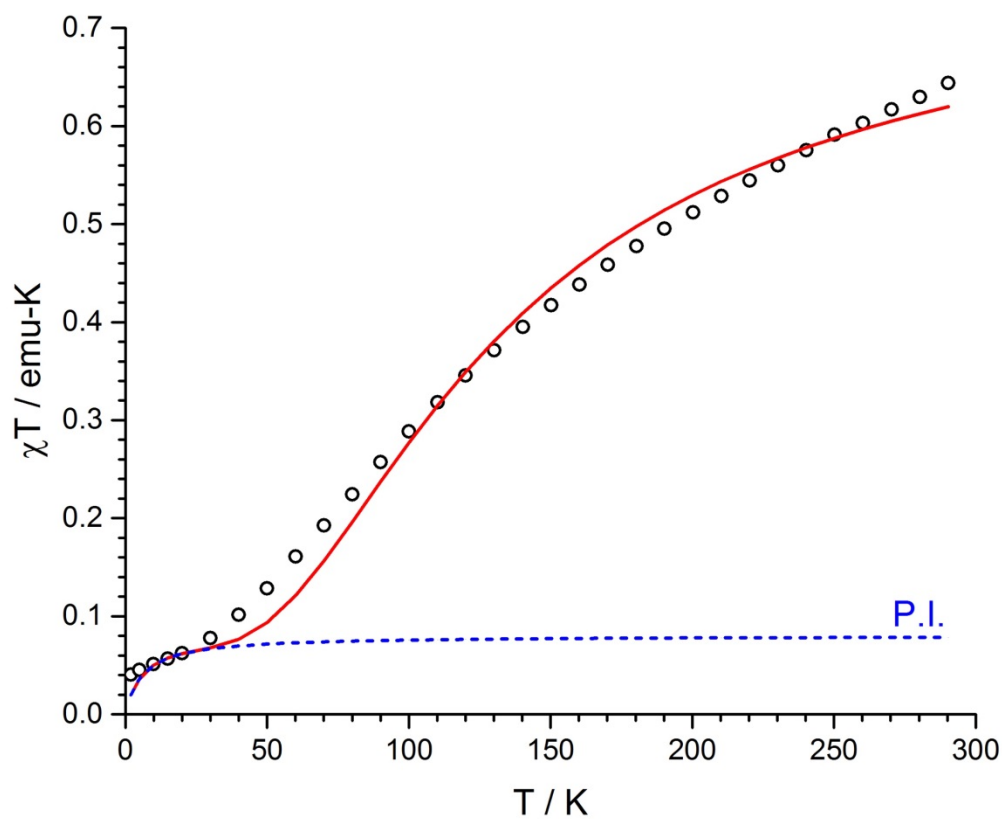

Figure S3. SQUID magnetometry data of *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] (open circles) along with simulated data (red line) and paramagnetic impurity (blue line). Fit parameters: J = -84.2 cm^{-1}; g$_1$ = g$_2$ = 2.039 (fixed); P.I. = 8.0% S = 1; T.I.P. = -471•10^{-6} emu; θ on TIP = -6 K; χ_{dia} = -1000 emu.

Section B. Synthetic and Calorimetric Studies.

General Methods. Unless stated otherwise all reactions were carried out inside an MBraun or Vacuum Atmospheres glovebox or utilizing Schlenk tube techniques under inert atmosphere conditions. Solvents were purified by distillation under argon from an appropriate drying agent into flame dried glassware. NMR spectra were recorded on either a Bruker 400 MHz or a Bruker 300 MHz NMR spectrometer. Pd-NHC complexes and their O_2 derivatives were prepared by methods strictly analogous to those reported previously.[2,3] Representative procedures for preparation and reactions of new complexes are described below.

NMR Studies of Reaction of [Pd(IPr)]$_2$ and O$_2$ at Room Temperature. A solution of 5 mg [Pd(IPr)$_2$] was weighed into an NMR tube in the glove box and dissolved in 0.5 mL C_6D_6 fitted with a screw cap and Teflon-lined silicone rubber septum. An NMR spectrum was taken and then 3 mL of pure O_2 gas was added to the tube and it was shaken. A second NMR spectrum recorded 16 minutes later showed complete disappearance of the signals due to the diamagnetic starting material and conversion to a paramagnetic product as shown in Figure S4a. ^{1}H NMR (400MHz, C_6D_6): δ = 7.16 (t, under peak of C_6D_6 at 7.16ppm, 4H), 6.65 (s, broad, 8H), 6.11 (s, broad, 4H), 3.29 (s, very broad, 32H), 1.67 (s, broad, 24H). The spectrum of starting material [Pd(IPr)$_2$] and product *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] are shown as an overlay in Figure S4b.
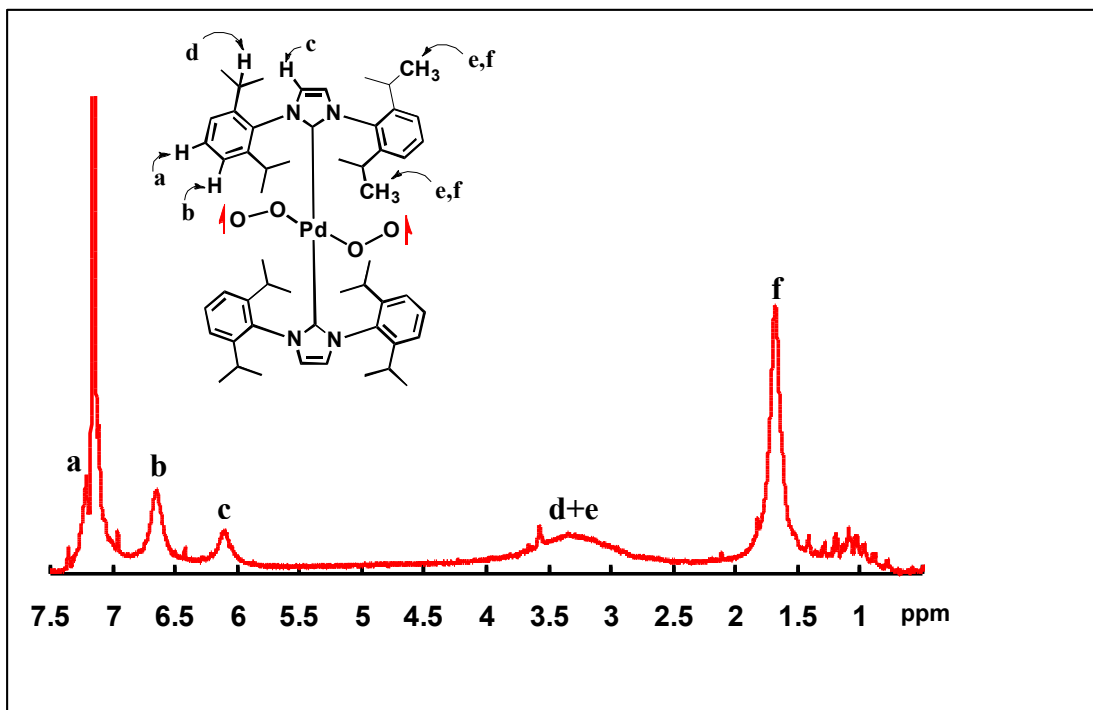
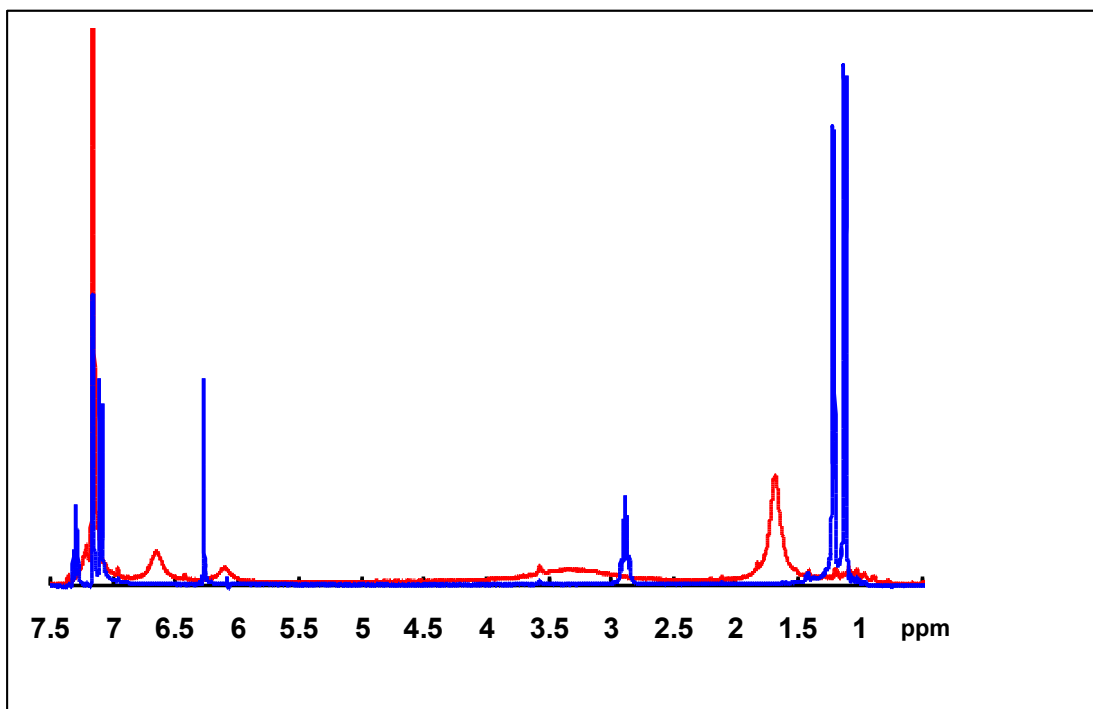**Figure S4a.** ^{1}H NMR spectrum in C_6D_6 of *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$].

Figure S4b. ^{1}H NMR spectrum in C_6D_6 of [Pd(IPr)$_2$] before addition of O$_2$ (blue spectrum) and after addition of O$_2$ (red spectrum). The red spectrum has been multiplied by 4 due to its broad nature.

B. Low-Temperature NMR study on O$_2$ binding to [Pd(IPr)$_2$]. In an NMR tube 8 mg [Pd(IPr)$_2$] was dissolved in 1 mL of tol-d^8 inside the glovebox. Then the tube was brought out of the glovebox and put into a Bruker 400 MHz NMR spectrometer, which was tuned to -70 ºC and equilibrated for 10min. When the temperature of the solution in the NMR tube was at -70 ºC and steady for 10min, a spectrum was taken for the stock solution. Then pure excessive O$_2$ was introduced by a tight syringe and the tube was shaken to make sure of good mixing. The tube was then put back into the NMR machine and waited until its temperature reached -70 ºC and steady for 10min. A series of NMR spectrum were run at the temperature range of -70 ºC to 20 ºC as shown in Figure S5
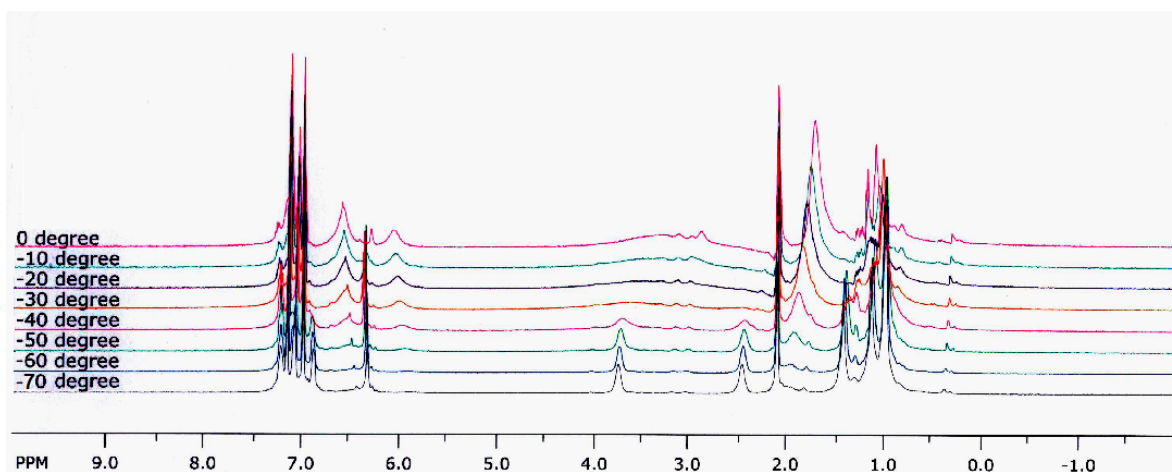
Figure S5. Low-T NMR spectra of adding O$_2$ to tol-d^8 solution of [Pd(IPr)$_2$] at variable temperatures.

Reversible O$_2$ Binding to [Pd(IPr)$_2$] at Low Temperature. 5 mL [Pd(IPr)$_2$] toluene solution of 0.0045M (20mg [Pd(IPr)$_2$]) was made and filled in a Schlenk tube in the glovebox. The tube was brought out of the glovebox and cooled down to -78 ºC in a dry ice/acetone bath until the temperature was stable, followed by introduction of excess O$_2$. The tube was shaken with the solution part emerged in the bath all the time to keep it at -78 ºC. The color of [Pd(IPr)$_2$] solution faded from fluorescent yellow-orange color to light yellow in less than 2 min. Then vacuum was applied to the tube and it was taken out of the bath. The tube was shaken and kept

under vacuum while warming up. The light yellow color turned back to yellow orange in less than 2min. This whole O_2 addition/vacuum procedure was repeated 10 times. In the end the [Pd(IPr)$_2$] solution was dried up under vacuum and an NMR spectrum was taken for its C_6D_6 solution.

Synthesis of [Pd(IPr)$_2$(OOH)(OH)]. 60 mg of [Pd(IPr)$_2$] was dissolved in 8 mL Et$_2$O and the solution was filled into a Schlenk tube inside the glovebox. The tube was then brought out of the glovebox and cooled down to -78 ºC in a dry ice/acetone bath until the temperature was stable, followed by introduction of excess O_2. The color of [Pd(IPr)$_2$] solution faded from fluorescent yellow-orange color to light yellow in less than 2min. Then vacuum was carefully applied to the tube at -78 ºC without shaking in order not form any [Pd(IPr)$_2$]. A 4.5 mL mixture of MeOH/H$_2$O containing 4 mL MeOH and 0.5 mL H$_2$O was premade. Under Argon gas flow, 4 drops of this MeOH/H$_2$O mixture was added to the solution under -78 ºC. Off-white precipitates were observed immediately floating in the solution. The reaction mixture was kept under Ar at -78 ºC for 4h before it turned yellow/orange. The liquid part of the mixture was evacuated off and the remaining yellow-orange solid was dried under vacuum for 1h. The yield of the synthesis of [Pd(IPr)$_2$(OOH)(OH)] is 73.8%. Peaks assigned to [Pd(IPr)$_2$(OOH)(OH)]: ^{1}H NMR (300MHz, tol d^8): δ = 7.28 (t, 4H, *p*-Ar), 7.13 (d, 8H, *o*-Ar), 6.36 (s, 4H, backbone of IPr), 3.77 (s, 1H, OOH), 2.97 (hep, 8H, CH on ^{i}Pr), 1.12 (d, 24H, ^{t}Bu on ^{i}Pr), 0.98 (d, 24H, ^{t}Bu on ^{i}Pr), -4.71 (s, 1H, OH). See Figure S6.
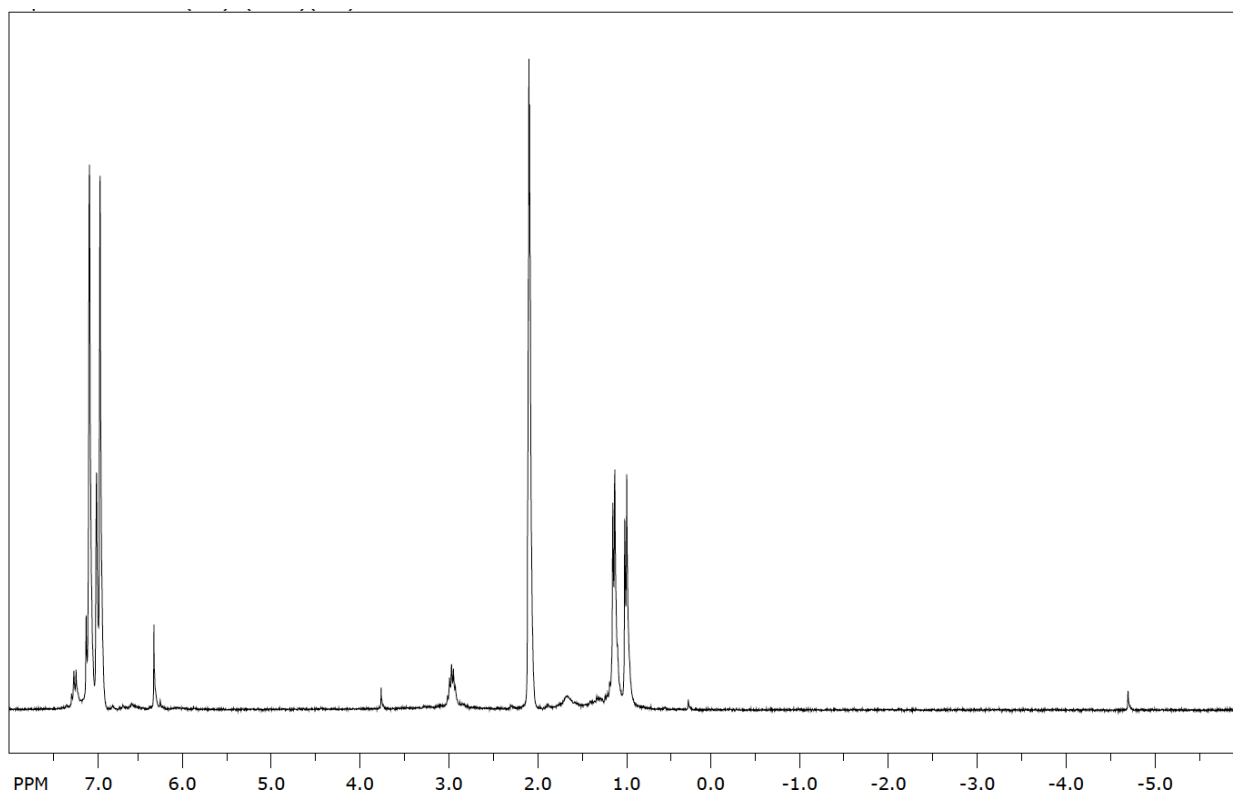
Figure S6. ^{1}H NMR spectrum in tol-d^8 of [Pd(IPr)$_2$(OOH)(OH)].

Synthesis of [Pd(IPr)$_2$(OOD)(OD)]. In an NMR tube, 5 mg [Pd(IPr)$_2$(OOH)(OH)] was dissolved in 1 mL tol-d^8. An NMR spectrum was taken at room temperature of this solution. Peaks at 3.77 ppm and 2.97 ppm show the presence of hydroxide and hydroperoxide groups. 1 drop of D$_2$O was added to the same NMR tube by pipette and NMR spectrum was taken again. The disappearance of these two peaks shows the replacement of H by D.

Controlled Experiments of H$_2$O with [Pd(IPr)$_2$(η^2-O$_2$)] and [Pd(IMes)$_2$(η^2-O$_2$)]. 7 mg [Pd(IPr)$_2$] was dissolved in 3 mL toluene and the solution was filled into a 25 mL Schlenk tube. Then the procedure described above in synthesis of [Pd(IPr)(OOH)(OH)] was followed. An NMR spectrum was run for the final product and confirmed it was [Pd(IPr)$_2$(OOH)(OH)].

7.3 mg [Pd(IMes)$_2$(η^2-O$_2$)] was dissolved in 3 mL toluene and exactly the same procedure was followed. An NMR spectrum was run for solid left after vacuum and drying. The

starting material $[Pd(IMes)_2(\eta^2\text{-}O_2)]$ was retrieved and there was no evidence that any other products were made.

Solution Calorimetric Measurements of Reaction of [Pd(IPr)₂] and O₂ in Toluene. Measurements of enthalpies of binding of $[Pd(IMes)_2]$ and $[Pd(IPr)(P\text{-}p\text{-}tolyl)_3]$ were made using Calvet calorimetric techniques strictly analogous to those reported previously.[3] The enthalpy of formation of *trans*-$[Pd(IPr)_2(\eta^1\text{-}O_2)_2]$ were made using an isoperibol Guild solution calorimetric system modified to work under O_2 atmosphere. In a Schlenk tube 350 mL of freshly distilled and purified anhydrous toluene was evacuate and filled with O_2 gas for three purge cycles and stirred for thirty minutes to ensure saturation. The calorimeter itself was purged with O_2 and under an outflow of O_2 the toluene solution was added. A small over-pressure of toluene was maintained by slow bubbling of dry O_2 gas through a T-tube fitted with a release bubbler filled with high vacuum silicone oil and attached to the calorimeter but in thermal isolation to prevent baseline drift. In the glove box 10 mL of a toluene solution containing a weighed sample of $[Pd(IPr)_2]$ (in the range 0.1 to 0.4 grams) was added to a 15 mL pipet in which one end had been rounded off and blown out to make a fragile glass bulb. A compression fitting adapter on the other pipet stem allowed immersion of the sample into the calorimeter. The open top end of the pipet which was outside the calorimeter assembly was connected by butyl-rubber thick walled tubing to a 10 mL Hamilton gas tight syringe which was filled initially with 10 mL of Argon gas. This apparatus was taken from the glove box and the sample immersed in the calorimeter solution under a flow of O_2 gas. After thermal equilibration a series of electrical calibrations were performed and the ampoule was broken by crushing it against a glass anvil on the bottom of the calorimeter. Immediately following the breaking of the ampoule the 10 mL of Argon gas was added to push the solution from the broken ampoule into the 350 mL of O_2 saturated toluene in the calorimeter.

Following return to baseline a second set of electrical calibrations were performed. Testing the solution by breaking ampoules prepared in identical fashion but containing no [Pd(IPr)$_2$] only 10 mL toluene yielded no detectable thermal signal. Reported data are the average of eight separate measurements.

Section C. Kinetic and Modelling Studies

Stopped-Flow Kinetics. Anhydrous toluene (HPLC grade, $\geq$ 99.9%) was purchased from Sigma Aldrich and dried on an Innovative Technologies PureSolv 400 solvent purification system. Toluene solutions of [Pd(IPr)$_2$] or [Pd(IMes)$_2$] were prepared in an MBraun glove box filled with ultra-high purity argon (Airgas) and loaded in Hamilton gastight syringes equipped with three-way valves. Saturated solutions of O$_2$ (Airgas, ultra-dry grade) were prepared by bubbling gas into gastight syringes containing dry toluene for at least 20 minutes; dilutions of the O$_2$ saturated solvent were performed anaerobically to obtain the desired [O$_2$] before mixing. The solubility of O$_2$ in toluene was taken as 8.3 mM at 20 °C.[4] Time resolved spectra (λ = 400−700 nm) were acquired over a range of temperatures (−85 to +25 °C) using a Hi-Tech Scientific KinetAsyst SF-61DX2 CryoStopped Flow system (TgK Scientific Ltd.) equipped with a quartz tungsten halogen light source, a J&M TIDAS diode array detector and a Brandenburg 4479 Series PMT monochromator. The instrument was equipped with stainless steel plumbing lined with PEEK tubing and a 1.00 cm^3 quartz mixing cell submerged in an ethanol cooling bath. The temperature in the mixing cell was maintained to ± 0.1 °C using a CAL 3200 automatic temperature controller. Data acquisition was performed using TIDAS-DAQ and/or Kinetic Studio software programs and mixing times were 2 - 3 ms. Reactions were studied under pseudo-first order conditions using excess O$_2$ whenever possible. Accurate measurements of the observed rate constants for these rapid binding processes are better performed using single

wavelength detection, and once the overall spectral features were examined, single wavelength measurements were utilized to quantify rate constants for the reactions at variable concentrations and temperatures. All flow lines were washed extensively with argon saturated dry toluene prior to loading reactant solutions. All experiments were performed in a single-mixing mode of the instrument with a 1:1 (v/v) mixing ratio. All concentrations are reported after mixing in the stopped flow cell. Data analysis was performed using Kinetic Studio, IGOR Pro 5.0 (Wavemetrics, Inc.), and ReactLab Kinetics Global Analysis software (JPlus Consulting Pty. Ltd.). All reported observed rate constants represent an average of three to seven measurements which gave an acceptable standard deviation (within 5 - 10 %) and all remaining quantities derived from the kinetic data are reported with their standard deviations.

Reaction of O_2 with [Pd(IMes)$_2$] in toluene solution at −80 °C proved too rapid to follow quantitatively by conventional stopped-flow techniques (Figures S7 and S8). It can be seen that near total bleaching of color (Figure S9) is observed within milliseconds. The extremely rapid reaction of [Pd(IMes)$_2$] with O_2 is in keeping with a very low activation energy for conversion to [Pd(IMes)$_2$(η^2-O_2)]. Attempts to monitor this rapid decay in single wavelength mode (λ = 458 nm) were conducted at −80 °C with varying [O_2] (0.10-0.83 mM after mixing) in an effort to obtain the second-order rate constant (k_{on}) for the binding of O_2 at low temperatures (Table S1). The only conclusion that can be drawn from the data is that $k_{on} \geq 10^6$ M^{-1} s^{-1} for O_2 binding to [Pd(IMes)$_2$] at −80 °C.
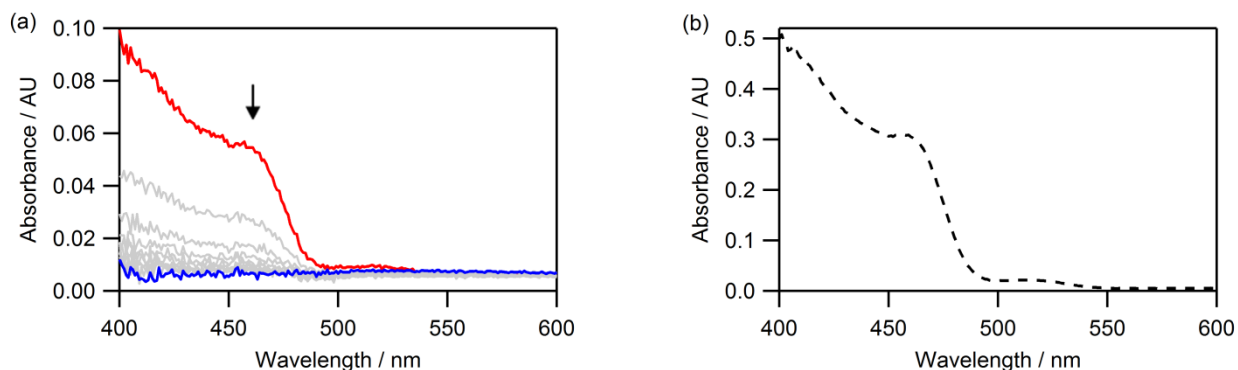
Figure S7 (a) Time-resolved spectral changes accompanying the reaction between [Pd(IMes)$_2$] (0.1 mM) and O$_2$ (0.1 mM) at −80 °C acquired over 3 s. Selected traces are shown for clarity. The initial time = 0 s trace is shown in red; gray traces were acquired at 0.003 s intervals and the final spectrum after 3 s reaction is shown in blue. (b) Absorbance spectrum of 0.1 mM [Pd(IMes)$_2$] in toluene highlighting its shoulder peak at λ ≈ 458 nm with ε ≈ 3,090 M^{-1} cm^{-1}. Most of the spectral decay that occurs upon O$_2$ binding happens within the instrument dead time of 2 - 3 ms and is therefore not resolvable with diode array detection.
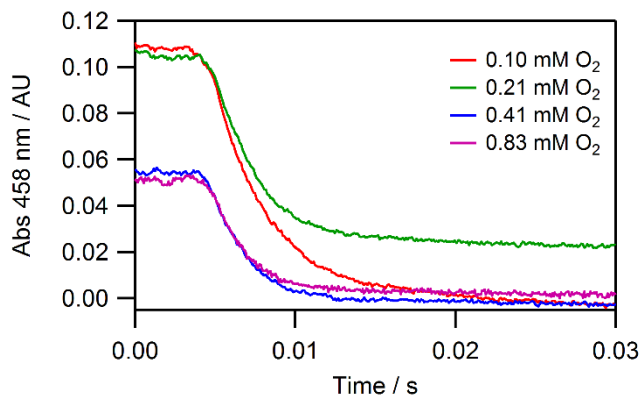
Figure S8. Single wavelength kinetic traces at λ = 458 nm as a function of [O$_2$]$_0$ obtained from the stopped-flow reaction of [Pd(IMes)$_2$] with O$_2$ at −80 °C.
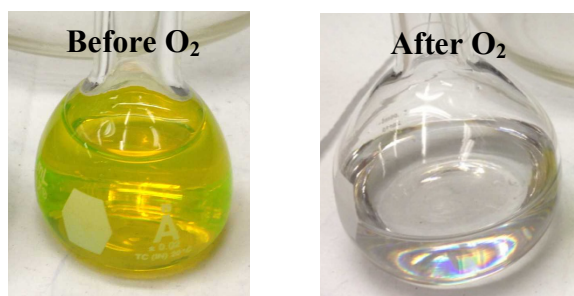
Figure S9. Comparison of toluene solutions of Pd(IMes)$_2$ (1 mM) before (left) and immediately after (right) exposure to O$_2$ at ambient temperature.

Table S1. Pseudo-first order (k_{obs}) rate constants for O$_2$ binding to [Pd(IMes)$_2$] (0.1 mM) at −80 °C. Kinetic traces were fit to a single exponential equation, y = −A*exp(−k_{obs}t) + C or y = −A*exp(−k_{obs}t) +Mx + C. The average value taken from multiple datasets is reported with the standard deviation. Since the reaction is so rapid, it is not possible to obtain an accurate reaction order with respect to [O$_2$]; instead, an estimate for the presumed second order rate constant (k_{on}) was made from the stoichiometric reaction as shown.

−80 °C	[O$_2$] (M)	k_{obs} (s^{-1})	k_{on} (M^{-1} s^{-1})
	0.10	270 ± 15	= k_{obs}/[O$_2$] ≈ 3 × 10^6
	0.21	340 ± 28	
	0.41	420 ± 13	
	0.83	480 ± 37	

Stopped-flow kinetic studies for the reaction of O$_2$ with [Pd(IPr)$_2$] were performed in toluene solution over a broad temperature range (−85 to +25 °C). Two types of spectral changes were observed: rapid bleaching at low temperatures (−85 to −70 °C) and formation of new absorption bands in the near-UV region at higher temperatures (−40 to +25 °C). The low temperature bleaching reaction revealed rapid decay of the starting complex as shown in Figure 3 (main text) without formation of new absorbance bands. This bleaching in color is rapid and similar to that observed for [Pd(IMes)$_2$] (Figures S7 – S9) but occurs on a time scale suitable for collection of quantitative data (Figure S10). At these low temperatures, formation of the orange-red bis-superoxo complex was not observed. Moreover, no spectroscopic evidence for an intermediate

such as $[Pd(IPr)_2(\eta^1\text{-}O_2)]$ was detected in these studies. Analysis of $[Pd(IPr)_2]$ decay traces at 473 nm (Figure S10) as a function of varying $[O_2]$ over the -85 to $-70°C$ temperature range revealed a systematic linear increase in the value of the observed rate constant, k_{obs} (Figure S11, Table S2), confirming a simple first order dependency on $[O_2]$ in the overall second order forward reaction involving O_2 binding (k_{on}) as shown in eq. S1

(S1)
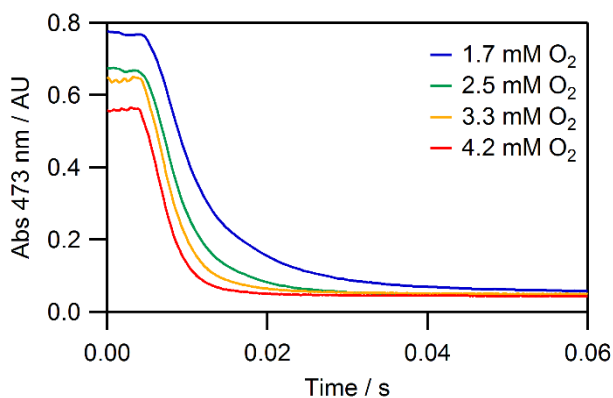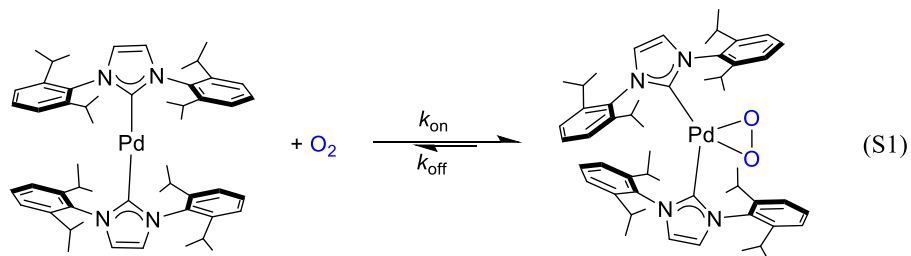
Figure S10. (a) $[Pd(IPr)_2]$ decay traces at $\lambda = 473$ nm acquired in single wavelength mode at -80 °C as a function of $[O_2]_0$.

Table S2. Temperature dependent pseudo-first order (k_{1obs} or k_{obs}) and second-order (k_{on}) rate constants for O_2 binding to [Pd(IPr)$_2$] (0.25 mM) at low temperatures, obtained from fitting decay traces ($\lambda = 473$ nm, decay) to a double exponential (at -85 °C only) or a single exponential equation (all remaining temperatures). Temperature dependent estimates of dissociation rates (k_{off}) are also provided.

-85 °C	[O$_2$] (M)	k_{1obs} (s^{-1})	k_{on} ($\times 10^4$ M^{-1} s^{-1})	k_{off} (s^{-1})
	1.7	97.2 ± 4.2		
	2.5	138 ± 9	4.36 ± 0.18	25 ± 5
	3.3	169 ± 13		
	4.15	206 ± 15		
-80 °C	[O$_2$] (M)	k_{obs} (s^{-1})	k_{on} ($\times 10^3$ M^{-1} s^{-1})	k_{off} (s^{-1})
	1.7	145 ± 12		
	2.5	193 ± 12	6.08 ± 0.14	42 ± 4
	3.3	246 ± 20		
	4.15	293 ± 38		
-75 °C	[O$_2$] (M)	k_{obs} (s^{-1})	k_{on} ($\times 10^3$ M^{-1} s^{-1})	k_{off} (s^{-1})
	1.7	206 ± 5		
	2.5	273 ± 4	8.46 ± 0.05	62 ± 2
	3.3	342 ± 8		
	4.15	413 ± 8		
-70 °C	[O$_2$] (M)	k_{obs} (s^{-1})	k_{on} ($\times 10^3$ M^{-1} s^{-1})	k_{off} (s^{-1})
	1.7	241 ± 3		
	2.5	353 ± 3	11.2 ± 0.7	61 ± 22
	3.3	437 ± 6		
	4.15	518 ± 2		
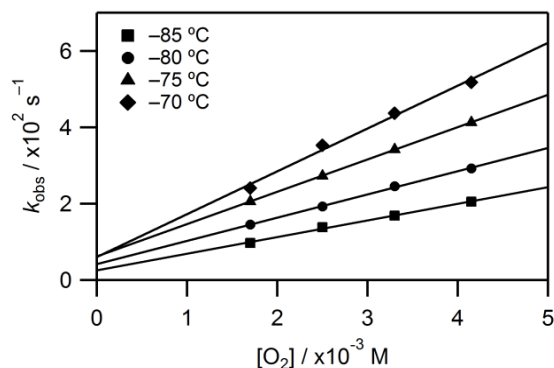
Figure S11. Plots of k_{obs} versus $[O_2]$ (markers) with linear fits (lines) for the reaction of O_2 with [Pd(IPr)$_2$]. Temperature range: −85 to −70 °C.
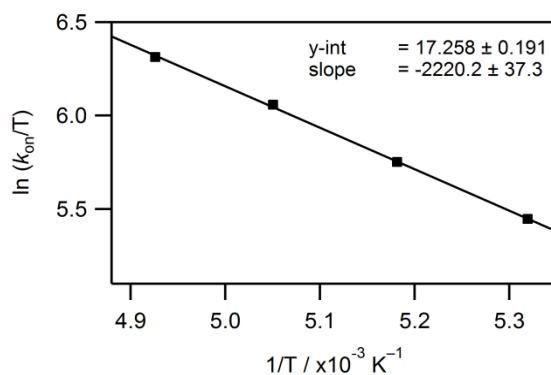
Figure S12. Eyring plot for the low temperature O_2 binding reaction to [Pd(IPr)$_2$].

The slopes of the linear plots (Figure S11) at low temperatures allowed for accurate determination of k_{on}; uncertainty in the intercepts, however, did not allow reliable quantitative evaluation of k_{off}. In general, the linear plots reveal an increase in the intercept as temperature increases, which would indicate that the equilibrium in eq. S1 is shifted to the right at lower temperatures. It is important to note that the accuracy in k_{off} values is typically low, and because the reaction is already extremely fast and nearing the limits of measurement, we regard these values as loose estimates. Furthermore, due to the large difference in the relative magnitudes of

k_{on} versus k_{off} (see Table S2), the dissociation reaction can be neglected, from the kinetic standpoint, at these low temperatures. Rate constants (k_{on}) for the low temperature second order O_2 binding reaction are provided in Table S2. The Eyring plot in Figure S12 yielded derived activation parameters of $\Delta H_1^{\ddagger} = 4.4 \pm 0.7$ kcal/mol and $\Delta S_1^{\ddagger} = -13 \pm 1$ cal/(mol·K).

Stopped Flow Kinetic Studies of Reaction of O_2 with $[Pd(IPr)_2]/[Pd(IPr)_2(\eta^2\text{-}O_2)]$ equilibrium mixtures forming *trans*-$[Pd(IPr)_2(\eta^1\text{-}O_2)_2]$. Based on the findings from variable temperature NMR studies, additional stopped flow experiments of reaction of $[Pd(IPr)_2]$ with O_2 were performed at higher temperatures (−40 °C to +25 °C) at which *trans*-$[Pd(IPr)_2(\eta^1\text{-}O_2)_2]$ is formed, in an effort to probe the mechanism of formation of this unique adduct. Representative spectroscopic changes at several different temperatures are shown in Figure S13. Relatively slow decay (occurring over ≈ 10 minutes at 0 °C) of the absorption band assigned to the starting $[Pd(IPr)_2]$ complex ($\lambda \approx 473$ nm) was observed, accompanied by the formation of a new, broad spectral feature centered near 444 nm which corresponds to the *trans*-$[Pd(IPr)_2(\eta^1\text{-}O_2)_2]$ product. The intensity of the absorbance band of the starting $[Pd(IPr)_2]$ complex near $\lambda = 473$ nm in the spectra obtained immediately upon mixing (blue traces in Figure S13) show a smooth decrease in peak height as the temperature decreases from +20 °C and has nearly disappeared at −40 °C. The intensity of the same absorbance band at 473 nm also decreases as a function of O_2 concentration at each temperature (Figures S14 and S15a). This is consistent with the rapid equilibrium between $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ and $[Pd(IPr)_2]$ as shown in eq. S2. The fraction of essentially colorless $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ complex increases with increasing $[O_2]$ or decreasing temperature, while the fraction of the red-orange starting complex $[Pd(IPr)_2]$ concomitantly decreases. The appearance of isosbestic points that shift position depending upon $[O_2]$ and temperature also reflect the changes in the $[Pd(IPr)_2(\eta^2\text{-}O_2)]/[Pd(IPr)_2]$ ratio.
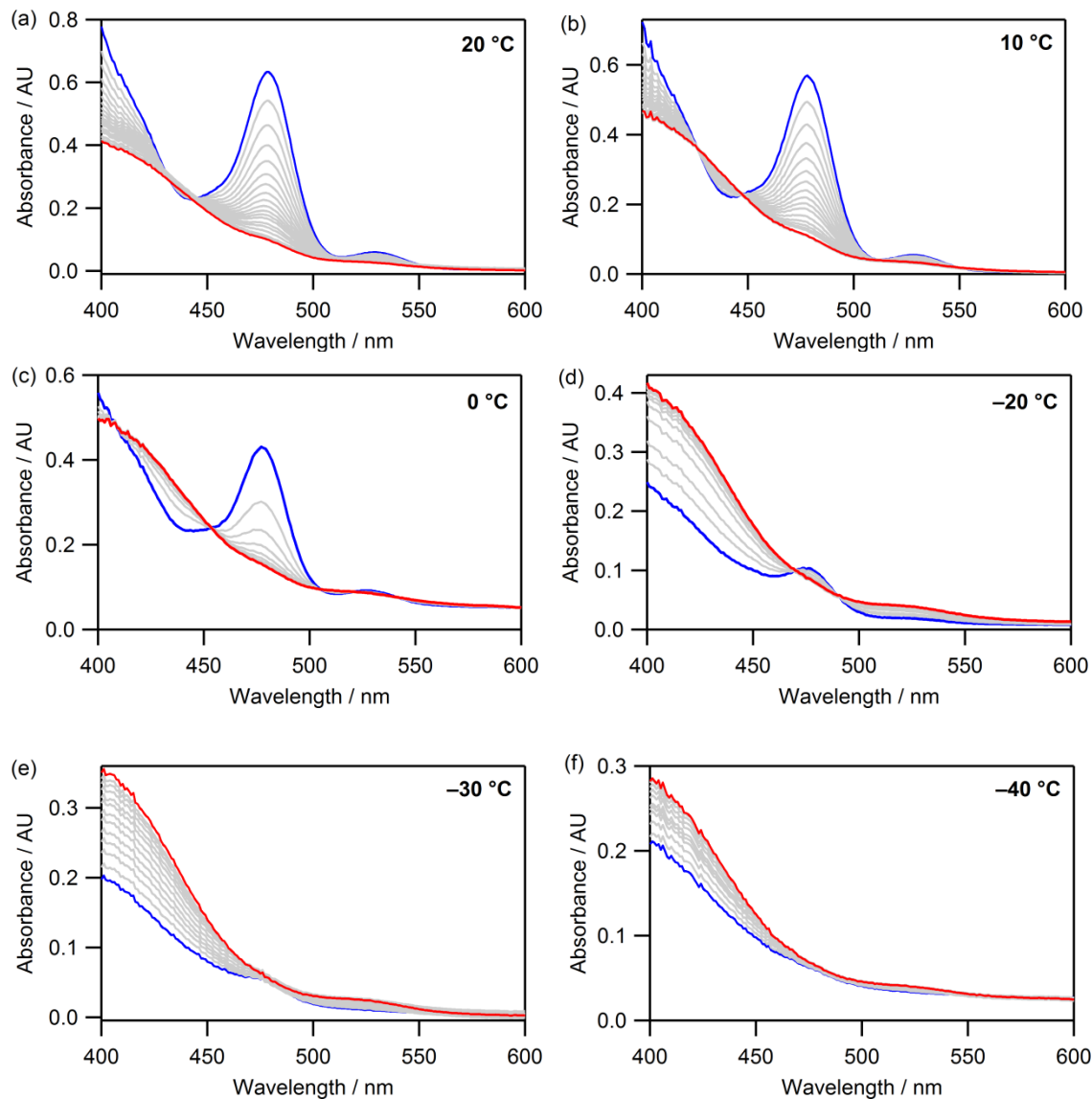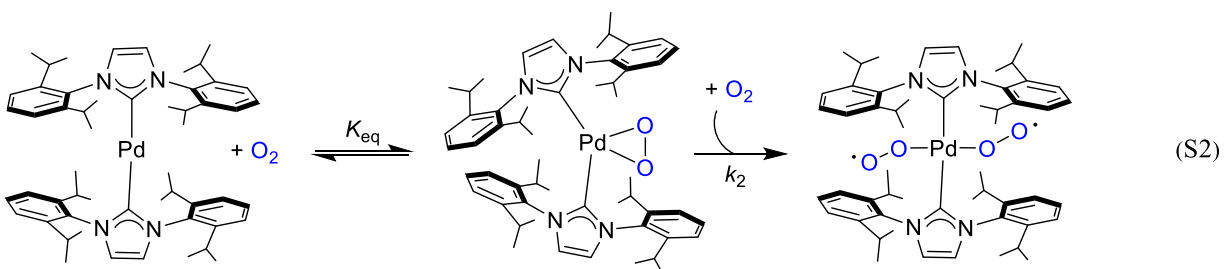
Figure S13. Time-resolved spectral changes for the reaction of [Pd(IPr)$_2$] (0.25 mM) with [O$_2$] (4.15 mM) at various temperatures: (a) 20 °C (630 s); (b) 10 °C (625 s); (c) 0 °C (600 s); (d) −20 °C (1005 s); (e) −30 °C (1200 s); (f) −40 °C (1200 s). In all cases, the initial time = 0 s traces are shown in blue and final traces in red. Selected traces are shown for clarity.
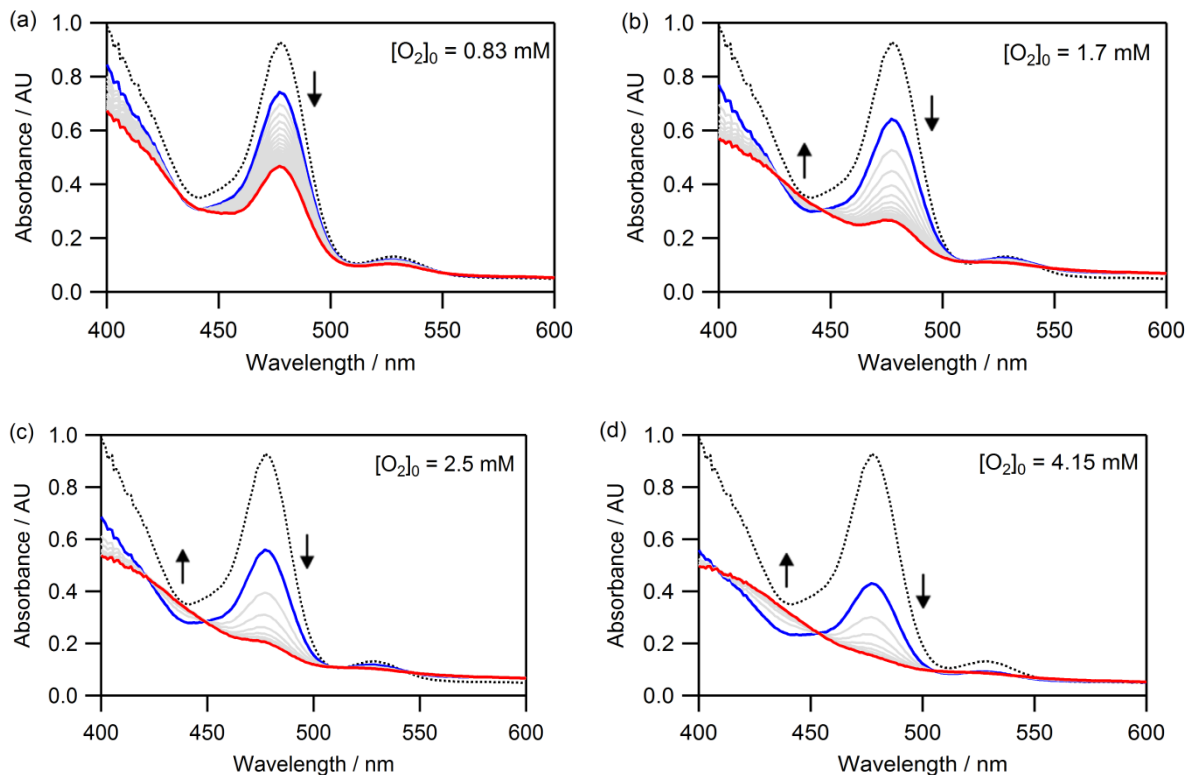
Figure S14. Time-resolved spectral changes for the reaction of [Pd(IPr)$_2$] (0.25 mM) with varying [O$_2$]$_0$ at 0 °C: In all cases, the initial time = 0 s traces are shown in blue and final traces in red. A spectrum of the starting [Pd(IPr)$_2$] complex at 0.25 mM (black dotted trace) has been overlaid to emphasize the attenuation of the initial absorbance values recorded upon initiation of the reaction with O$_2$.
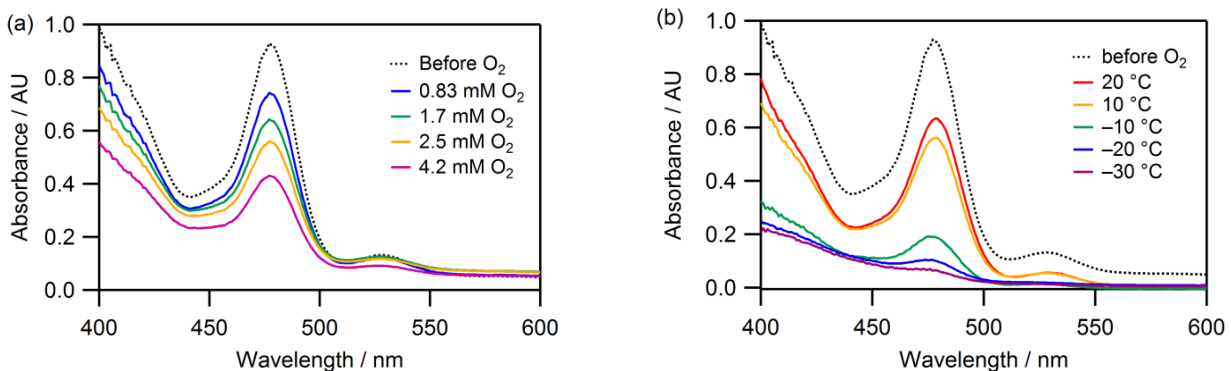
Figure S15. (a) Overlay of initial time = 0 s spectra acquired for reactions of [Pd(IPr)$_2$] with varying O$_2$ concentration at constant temperature (0 °C). (b) Overlay of initial time = 0 s spectra acquired for reactions of [Pd(IPr)$_2$] with O$_2$ at various temperatures at constant [O$_2$]$_0$ (4.15 mM after mixing).

The equilibrium constant associated with the first O_2 binding step was derived at various temperatures ($-20\ ^\circ$C to $+20\ ^\circ$C) directly from the experimental data using the initial absorbance values in reactions of $[Pd(IPr)_2]$ with variable concentrations of O_2 according to eq. S3. The nonlinear plot obtained from fitting data at 20 $^\circ$C to eq. S3 is shown in Figures S16 and S17. Values of the equilibrium constant are summarized in Table S3.

A van't Hoff plot provided the thermodynamic parameters for O_2 binding to form $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ ($\Delta H = -14 \pm 1$ kcal/mol; $\Delta S = -40 \pm 3$ cal/(mol·K)) as shown in Figure S18).

$$A_0 \text{ (478 nm)} \ = \ \frac{\epsilon [Pd(IPr)_2]_0}{(1 + K_{eq}[O_2]_0)} \qquad\qquad \text{(S3)}$$
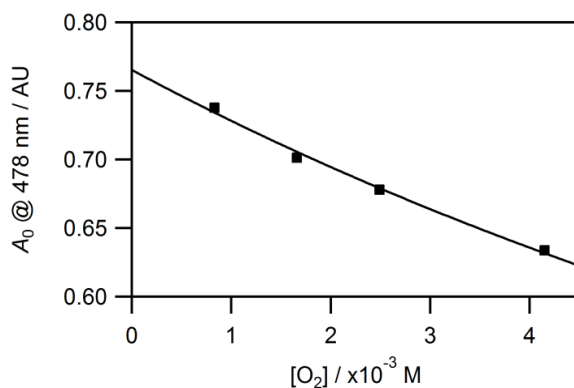
Figure S16. Plot of initial absorbance ($\lambda = 478$ nm) versus $[O_2]_0$ (markers) at 20 $^\circ$C with nonlinear fit to eq. S3 (solid line). The derived value of K_{eq} at this temperature is 51 ± 3.
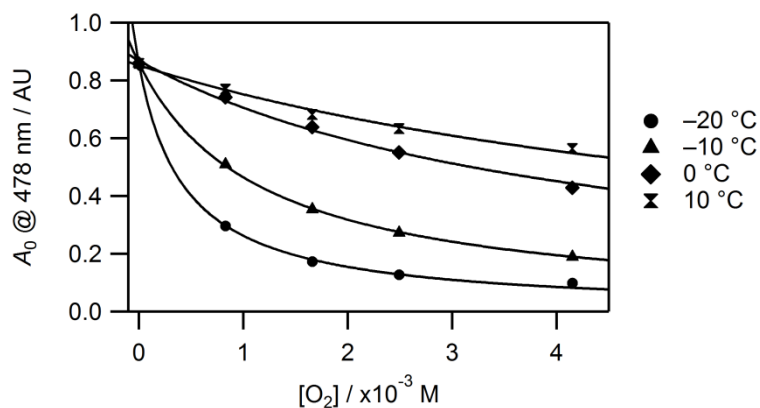
Figure S17. Plots of initial absorbance (A_0 at $\lambda = 478$ nm) versus $[O_2]_0$ (markers) at various temperatures with non-linear fits to Eq. S3 (solid lines) from which K_{eq} values were derived.

Table S3. Temperature dependent equilibrium constants (K_{eq}) derived from fitting plots of initial absorbance ($\lambda = 478$ nm) versus $[O_2]_0$ to the expression in Eq. S3. $[Pd(IPr)_2]_0$ was fixed at 0.25 mM. At 20 °C only, the first data point (at $[O_2] = 0$) was omitted.

T (°C)	K_{eq} (M^{-1})
+20	51 ± 3
+10	130 ± 10
0	230 ± 14
−10	850 ± 11
−20	$2{,}270 \pm 92$
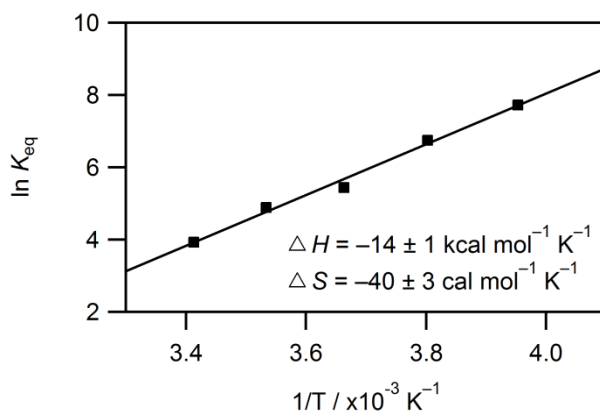
Figure S18. van't Hoff plot for O_2 binding to $[Pd(IPr)_2]$ to form $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ using experimentally derived values of K_{eq} (T range $= -20$ to $+20$ °C) with derived thermodynamic parameters.

Reaction rates for formation of *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] as a function of [O$_2$] could only be readily measured over a temperature range of −20 to +20°C since the process became exceptionally slow at lower temperatures. Observed rate constants, obtained from fitting the decay traces at λ = 478 nm, depend nearly linearly on [O$_2$] only at −20 °C; at higher temperatures the plots display curvature as shown in Figure S19. This ultimately reveals a more complicated reaction order with respect to [O$_2$]. In this case, it is evident that the overall reaction rate is not dominated by a single elementary step in the temperature range of 20 °C $\leq T \geq$ 0 °C.
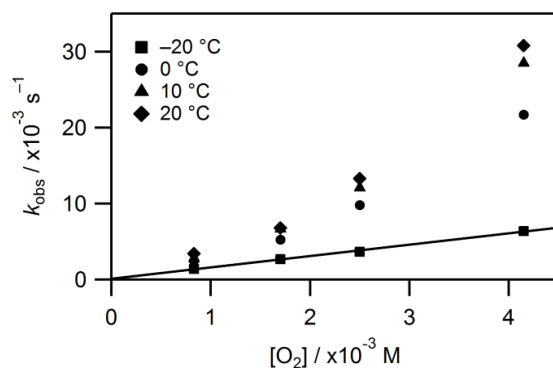
Figure S19. Plots of k_{obs} versus [O$_2$] obtained over the temperature range of −20 to 20 °C. A linear fit is shown for the −20 °C plot, which yielded a second order rate constant (k_2) of 1.50 ± 0.06 M^{-1} s^{-1} (R^2 = 0.997).

Assuming a rapid [Pd(IPr)$_2$]/[Pd(IPr)$_2$(η^2-O$_2$)] pre-equilibrium followed by rate limiting binding of the second O$_2$ molecule, the value of k_{obs} will obey eq. S4, a derivation of which is provided in the next section.

$$k_{obs} = \frac{K_{eq}k_2[O_2]^2}{1+K_{eq}[O_2]}$$
(S4)

Derived values for k_2 and K_{eq} obtained from eq. S4 are shown in Table S4. Plots of k_{obs} versus [O$_2$] with fits to eq. S4 are provided in Figure S20. As explained in the following section, these thermodynamic and kinetic parameters obtained from traditional treatment of single wavelength

absorbance changes at certain temperatures and reagent concentrations are in good agreement with full computer simulation of the time-resolved spectra using the ReactLab Kinetics program.

Table S4. Temperature dependent equilibrium constants (K_{eq}) for rapid pre-equilibrium formation of $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ and second order rate constants (k_2) for the formation of *trans*-$[Pd(IPr)_2(\eta^1\text{-}O_2)_2]$.

T (°C)	K_{eq}	k_2 ($M^{-1}\,s^{-1}$)
+20	51 ± 3^a	43 ± 2
+10	207 ± 88 $(130 \pm 10)^b$	15 ± 4
0	303 ± 130 $(230 \pm 14)^b$	9.3 ± 1.9
−20	^{c}	1.53 ± 0.03 $(1.50 \pm 0.06)^d$

^{a} K_{eq} value was fixed and taken from experimental data fit to Eq. S3 (see Figure S16-S17). ^{b} Values in parenthesis are those from experimental data fit to Eq. S3. ^{c} An accurate value could not be obtained from the nonlinear fit. ^{d} Value in parenthesis represents the result obtained from experimental data shown in Figure S17.

Derivation of Eq. S4 for analysis of high temperature [O₂] dependency plots.

Assumption 1: The $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ absorbance is so weak that it does not contribute to the measurement; the total concentration of Pd containing species can be expressed as follows:

$$[Pd(IPr)_2]_0 = [Pd(IPr)_2] + [Pd(IPr)_2(\eta^2\text{-}O_2)] + [Pd(IPr)_2(\eta^1\text{-}O_2)_2] \qquad (S5)$$

Taken in derivative form, and since $d[Pd(IPr)_2]_0 / dt = 0$, we know that:

$$\frac{d[Pd(IPr)_2]_0}{dt} = 0 = \frac{d[Pd(IPr)_2]}{dt} + \frac{d[Pd(IPr)_2(\eta^2\text{-}O_2)]}{dt} + \frac{d[Pd(IPr)_2(\eta^1\text{-}O_2)_2]}{dt} \quad (S6)$$

Rearranging to express in terms of product formation yields:

$$\frac{d[Pd(IPr)_2(\eta^1\text{-}O_2)_2]}{dt} = -\left(\frac{d[Pd(IPr)_2]}{dt} + \frac{d[Pd(IPr)_2(\eta^2\text{-}O_2)]}{dt}\right) \qquad (S7)$$

Assumption 2: The binding equilibrium is fast relative to all other observed steps; at all times we can assume the following:

$$K_{eq}[Pd(IPr)_2][O_2] = [Pd(IPr)_2(\eta^2\text{-}O_2)] \qquad (S8)$$

Incorporating Eq. S8 into Eq. S7 yields:

$$\frac{d[Pd(IPr)_2(\eta^1\text{-}O_2)_2]}{dt} = -\frac{d[Pd(IPr)_2]}{dt}(1 + K_{eq}[O_2]) \qquad (S9)$$

Assumption 3: The rate law corresponds to a rapid pre-equilibrium initial binding step which is followed by a rate determining second step:

$$\frac{d[Pd(IPr)_2(\eta^1\text{-}O_2)_2]}{dt} = -\frac{d[Pd(IPr)_2]}{dt}\left(1 + K_{eq}[O_2]\right) = K_{eq}k_2[Pd(IPr)_2][O_2]^2 \qquad (S10)$$

Rearranging the above expression in terms of $[Pd(IPr)_2]$, since we are directly monitoring its decay:

$$-\frac{d[Pd(IPr)_2]}{dt} = \frac{K_{eq}k_2[Pd(IPr)_2][O_2]^2}{\left(1 + K_{eq}[O_2]\right)} \qquad (S11)$$

Upon integration, of Eq. S11, first order decay of $[Pd(IPr)_2]$ is observed under pseudo-first order conditions (excess O_2), and k_{obs} for this process will be eq. S12:

$$k_{obs} = \frac{K_{eq}k_2[Pd(IPr)_2][O_2]^2}{\left(1 + K_{eq}[O_2]\right)} \qquad (S12)$$
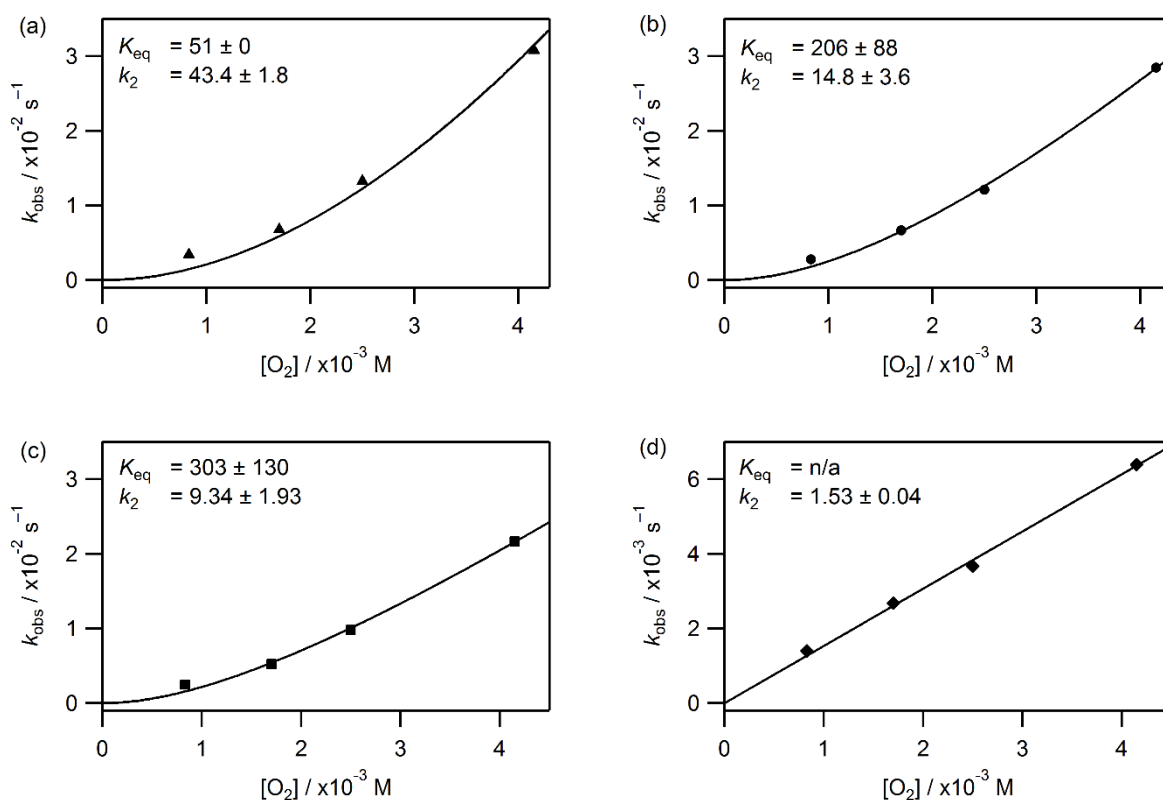
Figure S20. Plots of k_{obs} versus $[O_2]$ at various temperatures (markers) with fits to Eq. S12 (lines). (a) 20 °C, (b) 10 °C, (c) 0 °C, (d) −20 °C.

Kinetic Modeling of Formation of *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$]. Global modeling of the time-resolved spectra over a broad temperature range (-40 to $+20$ °C) to the mechanism provided in eq. S2 was performed using the ReactLab Kinetics program in an effort to validate the experimental analyses described in the previous section and determine the rate of formation of *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] over a broader temperature range. As discussed earlier, the first step of the reaction represents the equilibrium binding of the first O$_2$ molecule to form the intermediate mono-oxygenated [Pd(IPr)$_2$(η^2-O$_2$)] species, which does not absorb appreciably in the visible spectral range. The second step represents irreversible binding of the second O$_2$ molecule which leads to the formation of the final *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] product. The spectroscopic data showed clean isosbestic points and the concentrations of the three species [(Pd(IPr)$_2$], [Pd(IPr)$_2$(η^2-O$_2$)], and *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$] could be determined. The calculated UV-visible spectra and concentration profiles for the modeled reaction at 20 °C are shown below in Figure S21. Additional plots obtained at other temperatures are provided below in Figure S23.
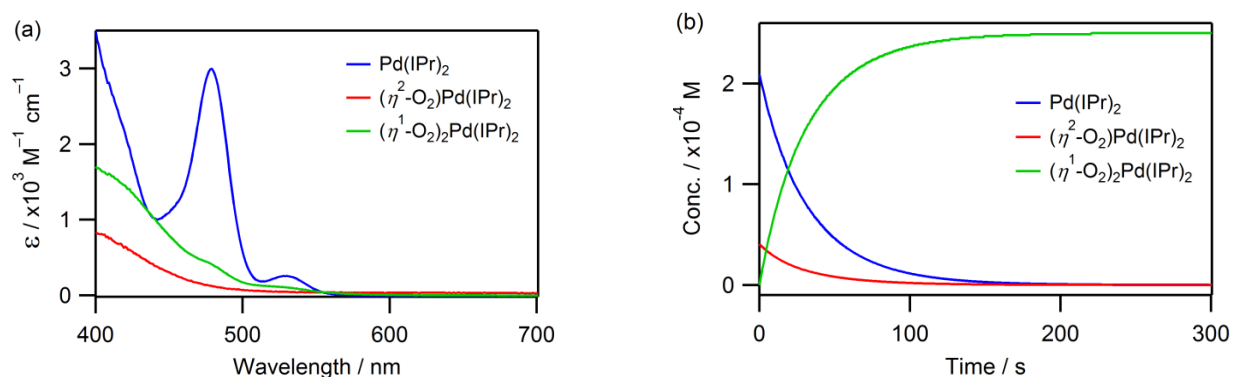
Figure S21. (a) Calculated UV-visible spectra of components obtained from the kinetic modeling at 20 °C. (b) Concentration profiles as a function of time. [Pd(IPr)$_2$]$_0$ = 0.25mM and [O$_2$]$_0$ = 4.15mM.

The modeled values of K_{eq} and k_2 were used to derive the thermodynamic (ΔH_1^0, ΔS_1^0) and activation parameters ($\Delta H_2^\ddagger$, $\Delta S_2^\ddagger$), respectively, associated with the two-step reaction in equation S2 as shown in Figure S22. Calculated equilibrium and rate constants are given in Table

S5 and are in good agreement with estimates obtained directly from the experimental analyses as shown in Table S4. In subsequent discussion, we adopt average values of $\Delta H_1^0 = -14.5 \pm 1.0$ kcal/mol and $\Delta S_1^0 = -43 \pm 3$ cal/(mol·K) for equilibrium binding of the first O_2 molecule to $[Pd(IPr)_2]$.
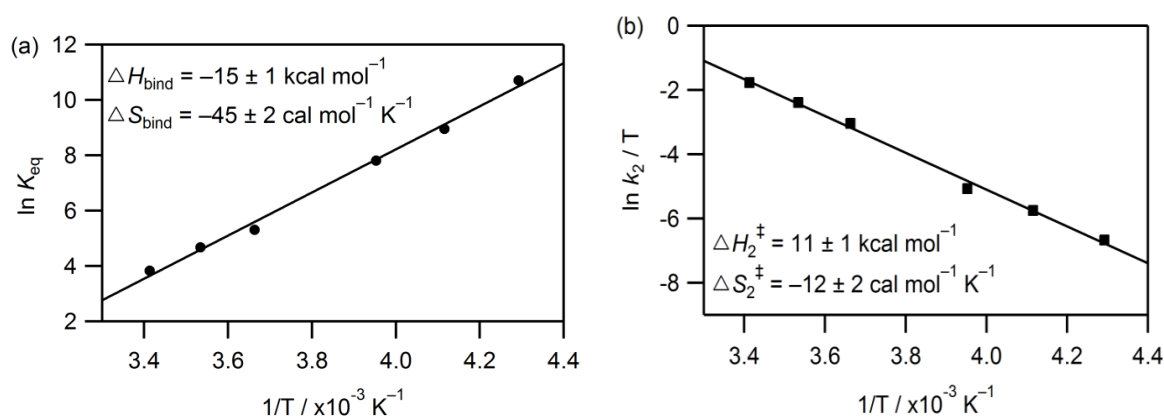
Figure S22. (a) van't Hoff plot constructed from the values of K_{eq} obtained from the kinetic model for equilibrium binding of O_2 to form $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ with derived thermodynamic parameters. (b) Eyring plot for formation of *trans*-$[Pd(IPr)_2(\eta^1\text{-}O_2)_2]$ from the monooxygenated adduct (k_2 step) with derived activation parameters.

The mechanism shown in eq. S2 shows approach to product occurring by attack of one O_2 molecule on the already formed $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ complex, which is in rapid equilibrium with $[Pd(IPr)_2]$ and free O_2. An alternate but kinetically equivalent route would assume that $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ is a dead-end complex which does not react with O_2 directly, but must first dissociate, fully or partially, to allow for the second O_2 molecule to approach the transition state (TS) en route to the *trans*-$[Pd(IPr)_2(\eta^1\text{-}O_2)_2]$ product. To take this into account, an alternative kinetic model was considered where dissociation of $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ was implied in the kinetic model by using a separate third order reaction involving the starting complex with two molecules of O_2 as shown in eq. S13.

(S13)
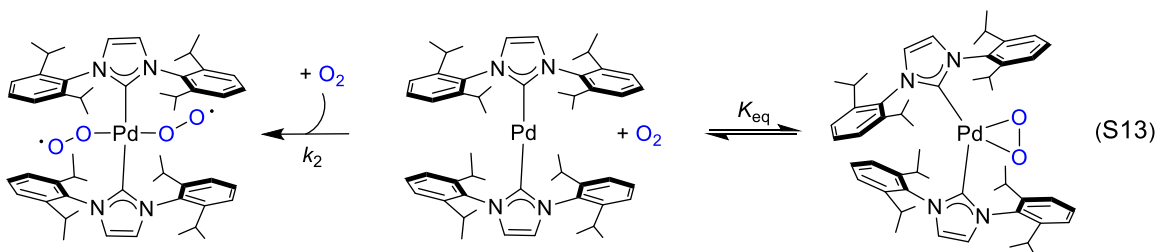
As shown below (Table S5), the values for the observed k_2 as well as activation parameters for this alternate reaction scheme obtained by kinetic modeling were identical to the appropriate values characterizing the reaction sequence in eq. S2. That is to be expected since kinetic data alone do not describe the nature of the TS, which may be approached from several different pathways. Specifically, the TS from $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ can be approached by full or partial dissociation, and since the binding and release of O_2 are much faster than all other steps this cannot be kinetically differentiated.

Table S5. Modeled values of rate and equilibrium constants for reaction S13 obtained from the kinetic model over a range of temperatures (−40 °C to +20 °C) with $[O_2]_0$ = 4.15 mM using ReactLab.[a,b] An average of two data sets is reported with standard deviations in all cases except at −30 and −40 °C, where only one data set is available. In those cases, the predicted standard deviation in k_2 was taken directly from the model and the error in K_{eq} is estimated at ± 30 %.

T (°C)	K_{eq} (M^{-1})	k_2 (M^{-1} s^{-1})
20	46 ± 1	50.5 ± 0.5
10	107 ± 2	25.9 ± 0.5
0[c]	202 ± 15	13 ± 1
−20	2,475 ± 85	1.59 ± 0.02
−30	7,730 ± 2,300	0.773 ± 0.001
−40	44,700 ± 13,400	0.295 ± 0.001

[a] The initial concentration of $[Pd(IPr)_2]$ was allowed to float; final calculated values ranged between 2.2 and 2.5 mM. [b] A known spectrum of $[Pd(IPr)_2(\eta^2\text{-}O_2)]$ obtained at −85 °C was incorporated at all temperatures. [c] The absorbance spectrum of the starting $[Pd(IPr)_2]$ complex was calculated by ReactLab to account for baseline shift; at all remaining temperatures, a known spectrum was used.
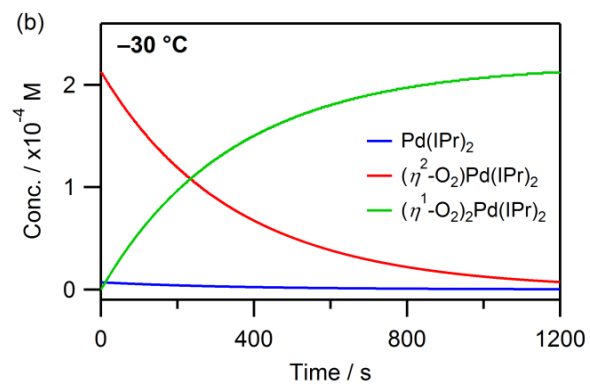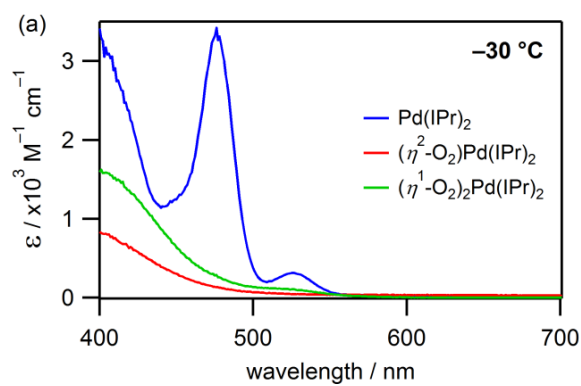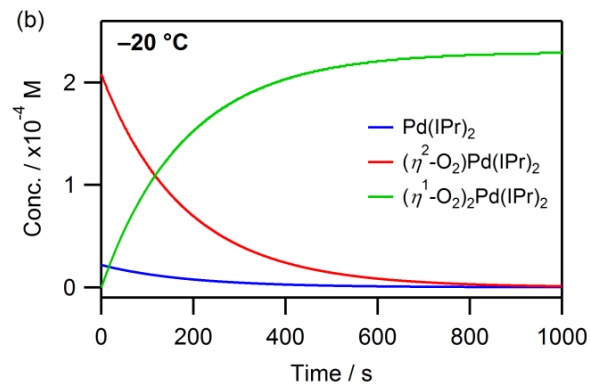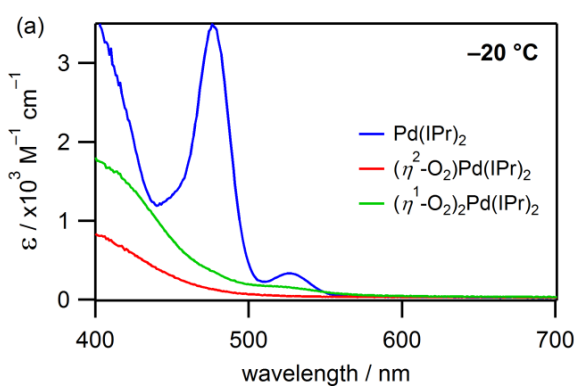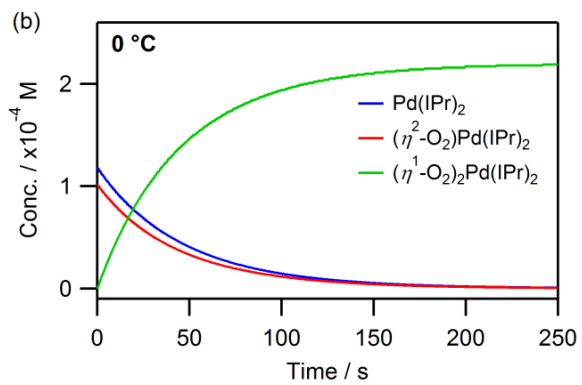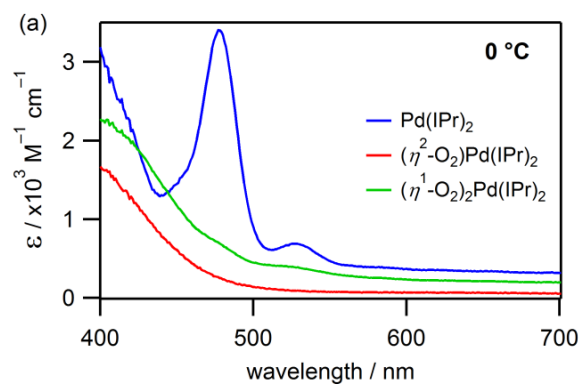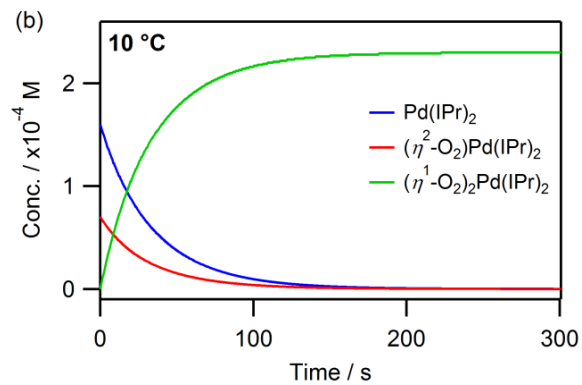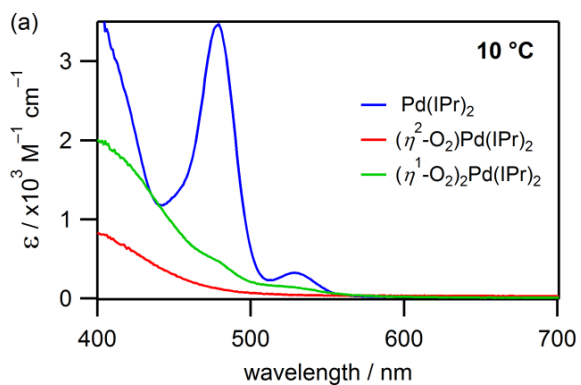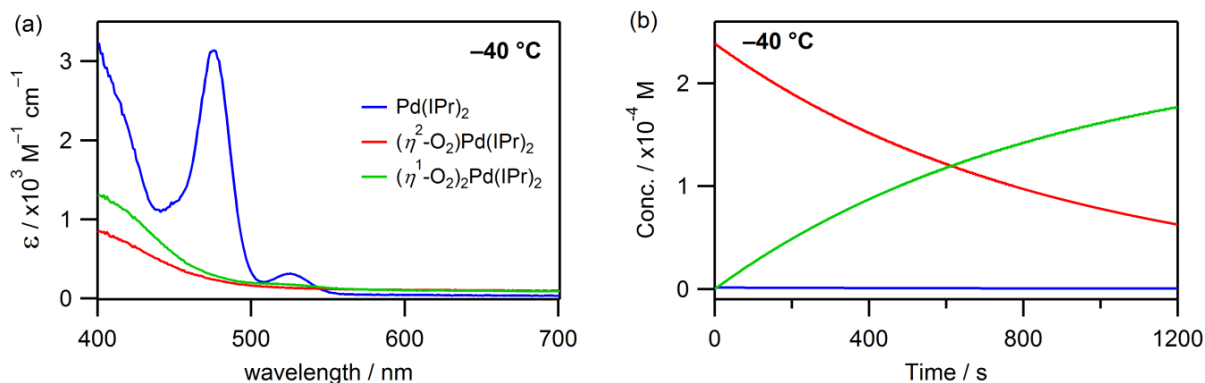
Figure S23. (a) Calculated spectra of colored components obtained from the kinetic model for the reaction S2 at temperatures of 10 °C, 0 °C, −20 °C, −30 °C, and −40 °C with $[Pd(IPr)_2]_0 = 0.22$ to 0.25 mM and $[O_2]_0 = 4.15$ mM. A known spectrum for $[Pd(IPr)_2]$ was incorporated in all cases except for 0 °C due to difficulties with baseline shifts. A known spectrum of $[Pd(IPr)_2(\eta^2-O_2)]$ was incorporated in all cases. The spectrum of $[Pd(IPr)_2(\eta^1-O_2)_2]$ was calculated by the fitting program in all cases. (b) Concentration profiles for colored components.

Section D. Crystal Structure Determination of *trans*-[Pd(IPr)₂(OOH)(OH)]

The data crystal of *trans*-[Pd(IPr)₂(OOH)(OH)] was glued onto the end of a thin glass fiber. X-ray intensity data were measured by using a Bruker SMART APEX2 CCD-based diffractometer using Mo Kα radiation (λ = 0.71073 Å).[5] The raw data frames were integrated with the SAINT+ program by using a narrow-frame integration algorithm.[5] Corrections for Lorentz and polarization effects were also applied with SAINT+. An empirical absorption correction based on the multiple measurement of equivalent reflections was applied using the program SADABS. All structures were solved by a combination of direct methods and difference Fourier syntheses, and refined by full-matrix least-squares on F^2, by using the SHELXTL software package.[6,7] Crystal data, data collection parameters, and results of the analyses are listed in Table S6. Compound *trans*-[Pd(IPr)₂(OOH)(OH)] crystallized in the monoclinic crystal system. The space group $P2_{1/c}$ was confirmed on the basis of the systematic absences in the data. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in geometrically idealized positions and included as standard riding atoms during the least-squares refinements.

Table S6. Crystallographic data for compound *trans*-Pd(IPr)$_2$(OOH)(OH)

Compound	*trans*-Pd(IPr)$_2$(OOH)(OH)
Empirical formula	PdO$_3$N$_4$C$_{54}$H$_{74}$
Formula weight	933.57
Crystal system	Monoclinic
Lattice parameters	
a (Å)	20.8909(9)
b (Å)	12.5657(5)
c (Å)	20.1842(9)
α (deg)	90
β (deg)	95.274(1)
γ (deg)	90
V (Å^3)	5276.1(4)
Space group	$P2_{1}/c$ (# 14)
Z value	4
ρ_{calc} (g / cm^3)	1.175
μ (Mo K$_a$) (mm^{-1})	0.394
Temperature (K)	296
$2\Theta_{max}$ (°)	52.0
No. Obs. (I > 2σ(I))	8430
No. Parameters	577
Goodness of fit GOF*	1.075
Max. shift in cycle	0.002
Residuals*: R1; wR2	0.0482; 0.1324
Absorption Correction, Max/min	Multi-scan 0.0482/0.1324
Largest peak in Final Diff. Map (e$^-$ / Å^3)	0.894

*R1 = $\Sigma_{hkl}(\mid\mid F_{obs}\mid - \mid F_{calc}\mid\mid)/\Sigma_{hkl}\mid F_{obs}\mid$; wR2 = $[\Sigma_{hkl}w(\mid F_{obs}\mid - \mid F_{calc}\mid)^2/\Sigma_{hkl}wF_{obs}^2]^{1/2}$,
w = 1/σ^2(F$_{obs}$); GOF = $[\Sigma_{hkl}w(\mid F_{obs}\mid - \mid F_{calc}\mid)^2/(n_{data} - n_{vari})]^{1/2}$.

Section E. Computational Studies

Unless stated otherwise, electronic structure calculations were performed using the PBE0 functional,[8] the D3(BJ) empirical dispersion correction[9] and the Def2-TZVP[10] basis set for Pd along with the corresponding ECP[11] and the 6-311G(d,p) basis set for the rest of the atoms. We refer to this basis set combination in this work as BSI. All stationary points were optimized by computing analytical energy gradients. The obtained minima were characterized by performing energy second derivatives, confirming them as minima or transition states by the number of negative eigenvalues of the Hessian matrix of the energy. To further refine the energies obtained from the PBE0-D3(BJ)/BSI calculations, single-point calculations in toluene solution using the IEF-PCM model[12] on the previously optimized gas phase structures were finally performed using the larger Def2-QZVP[10] and 6-311+G(2d,p) basis set for Pd and the rest of the atoms respectively. We refer to this basis set combination in this work as BSII. To check the influence of the functional, these single-point calculations were carried out with the PBE0,[8] B3LYP[13] and BP86[14] density functionals for selected species. To determine ΔH^0(298 K) and ΔG^0(298 K) values, computed electronic energies obtained using the larger BSII basis set were corrected for zero-point energy, thermal energy and entropic effects estimated from the normal mode analysis using the smaller BSI basis set. Strictly analogous calculations without the D3(BJ) empirical dispersion corrections[9] were also carried out for selected species to test their influence in the thermochemical values. In all calculations, the $<S^2>$ value was checked to confirm the electronic configuration of converged SCF wavefunctions (0, ≈1 and ≈2 for CSS, OSS and OST respectively). Spin projection corrections to OSS energies were performed as previously reported.[15] Calculations were performed with the Gaussian 09 suite of programs.[16]

As described above, several computational methods were tested in this work that can be referred as Functional-D3(BJ)(PCM)/BSII//PBE0-D3(BJ)/BSI and Functional(PCM)/BSII//

PBE0/BSI (Functional = BP86, PBE0, B3LYP). All of them, work reasonably well to describe superoxide species that contain a *trans* disposition of the NHC ligands. However, the majority of the methods fail to describe appropriately the thermochemistry of peroxides with a *cis* disposition of the NHC ligands. Enthalpies of O_2 binding lower than those obtained experimentally were computed using the hybrid functionals and with all functionals when empirical dispersion corrections were not included in the calculations, with deviation as large as 12-20 kcal/mol. The best agreement between calculated and experimental thermochemical values was obtained at the BP86-D3(BJ)(PCM)/BSII//PBE0-D3(BJ)/BSI level. Thus, unless stated otherwise, all energy values reported in the current work correspond to calculations at this level of theory.

To assess the reliability of the structural data obtained by DFT calculations, a comparison was made between complexes for which structural data were available. For *cis*-[Pd(IMes)$_2$(η^2-O$_2$)], *trans*-[Pd(IPr)$_2$(η^1-O$_2$)$_2$], *trans*-[Pd(IPr)$_2$(OOH)(OH)] and the parent [Pd(NHC)$_2$] complexes, there is good agreement between the optimized structures computed by DFT and those determined by X-ray crystallography (see Table S7) with differences generally lower than 0.02 Å and 4° in bond lengths and angles, respectively. One of the largest deviations is observed in the O-O bond length in *cis*-[Pd(IMes)$_2$(η^2-O$_2$)] for which the computed O-O distance of 1.383 Å compares to the experimental value of 1.443 Å. However, the energetic difference between the optimized structure of *cis*-[Pd(IMes)$_2$(η^2-O$_2$)] while constraining it to have the crystallographic Pd-O-O metrics and that of the fully optimized minimum was computed to be just 0.8 kcal/mol. The optimized structures of all peroxides and superoxides studied are shown in Figures S24-S27.

Table S7. Comparison between computational at the PBE0-D3(BJ)/BSI level and experimental (in red) selected metrical parameters (Average distances in Å and angles in degrees).

	O1–O2	Pd–O1	Pd–C	Pd–O1–O2	C–Pd–C
[Pd(IMe)$_2$]			2.013, 2.010		180.0, 180.0
[Pd(IMes)$_2$]			1.988, 1.990		180.0, 178.8
[Pd(IPr)$_2$]			2.023, 2.006		180.0, 178.5
[Pd(IMes)$_2$(η^2-O$_2$)]	1.383, 1.443	2.004, 2.010	2.022, 2.034	69.8, 69.0	111.0, 107.6
[Pd(IPr)$_2$(η^1-O$_2$)$_2$]	1.293, 1.327	2.021, 2.011	2.047, 2.062	117.0, 117.9	179.4, 178.2
[Pd(IPr)$_2$(OOH)(OH)]	1.485, 1.465	2.025, 2.009	2.032, 2.051	111.7, 111.1	178.9, 179.3
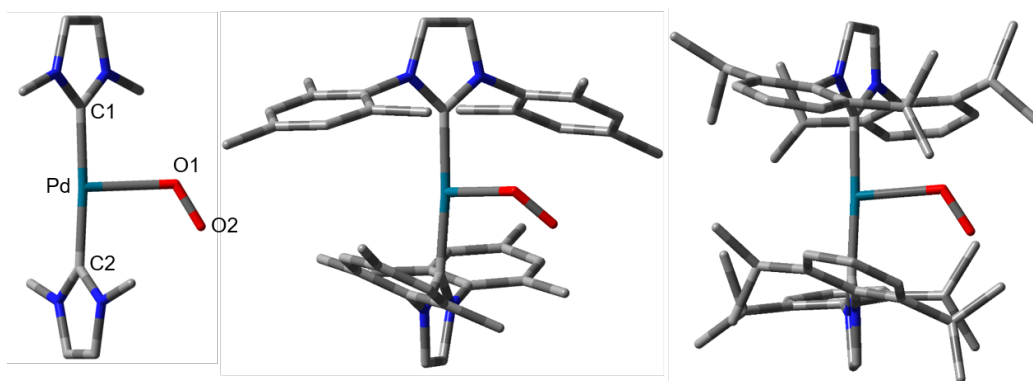
Figure S24. Optimized structures of the [Pd(NHC)$_2$(η^1-O$_2$)] complexes in the OST state. Selected metrical parameters (distances in Å and angles in degrees) for NHC = IMe (left), IMes (middle) and IPr (right): Pd-O1 = 2.341, 2.253, 2.229; Pd-O2 = 3.140, 3.059, 3.050; O1-O2 = 1.246, 1.263, 1.265; O1-Pd-O2 = 20.3, 21.3, 21.3; C1-Pd-C2 = 175.9, 173.6, 176.7. Hydrogen atoms omitted for clarity.
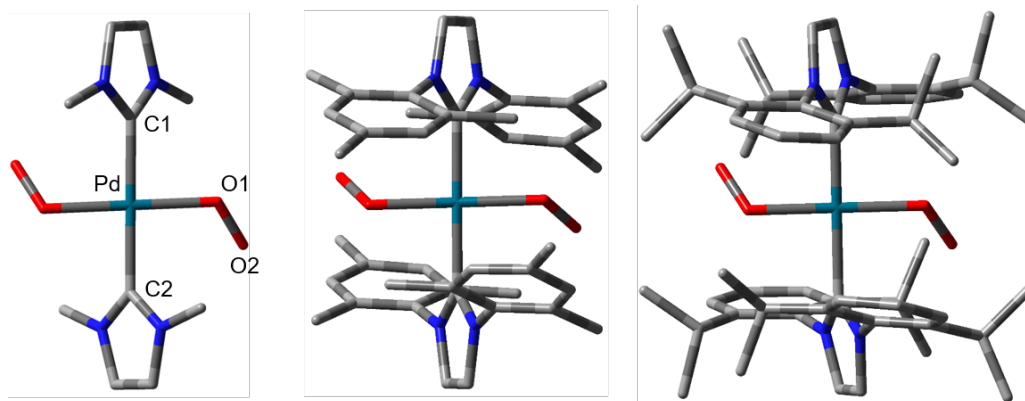
Figure S25. Optimized structures of the *trans*-[Pd(NHC)$_2$(η^1-O$_2$)$_2$] complexes. Selected metrical parameters (distances in Å and angles in degrees) for NHC = IMe (left), IMes (middle) and IPr (right): Pd-O1 = 2.037, 2.026, 2.021; O1-O2 = 1.294, 1.292, 1.293; O1-Pd-O2 = 23.7, 23.3, 23.8; C1-Pd-C2 = 178.9, 179.1, 179.4. Hydrogen atoms omitted for clarity.
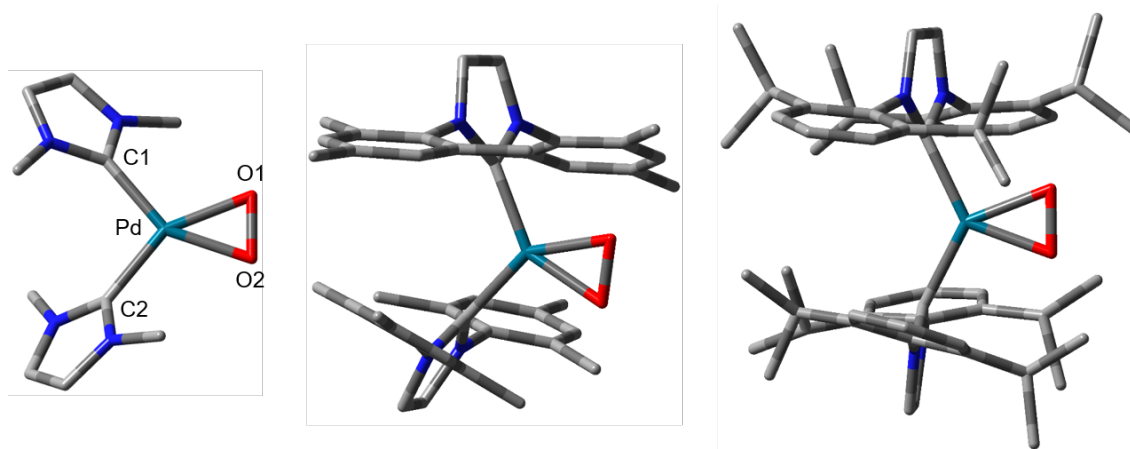
Figure S26. Optimized structures of the *cis*-[Pd(NHC)$_2$(η^2-O$_2$)] complexes. Selected metrical parameters (distances in Å and angles in degrees) for NHC = IMe (left), IMes (middle) and IPr (right): Pd-O1 = 1.993, 2.004, 2.003; O1-O2 = 1.388, 1.383, 1.374; O1-Pd-O2 = 40.7, 40.4, 40.1; C1-Pd-C2 = 101.9, 111.0, 125.2. Hydrogen atoms omitted for clarity.
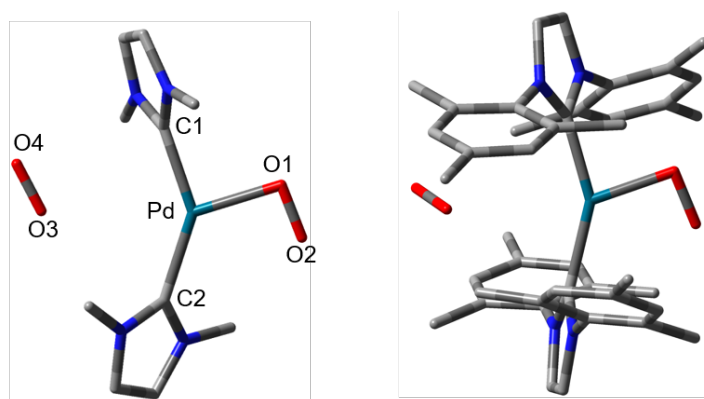
Figure S27. Optimized structures of the TS computed for addition of O$_2$ to *cis*-[Pd(NHC)$_2$(η^2-O$_2$)]. Selected metrical parameters (distances in Å and angles in degrees) for NHC = IMe (left), IMes (right): Pd-O1 = 2.111, 2.002; Pd-O3 = 3.450, 3.254; O1-O2 = 1.279, 1.318; O3-O4 = 1.199, 1.200; Pd-O1-O2 = 92.8, 92,2; Pd-O3-O4 = 116.3, 125.3; C1-Pd-C2 = 142.9, 150.9. Hydrogen atoms omitted for clarity.

Computed thermochemical parameters for the reactions forming the different peroxide or superoxide products by reaction of the parent [Pd(NHC)$_2$] complexes with O$_2$ as shown in equations S14-S16 are collected in Table S8.

$$[Pd(NHC)_2] + O_2 \rightarrow [Pd(NHC)_2(\eta^2\text{-}O_2)] \tag{S14}$$
$$[Pd(NHC)_2] + O_2 \rightarrow [^3Pd(NHC)_2(\eta^1\text{-}O_2)] \tag{S15}$$
$$[Pd(NHC)_2] + 2\ O_2 \rightarrow [Pd(NHC)_2(\eta^1\text{-}O_2)_2] \tag{S16}$$
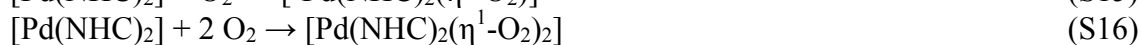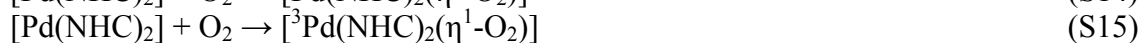
Table S8. Computed thermochemical values for selected equations. ΔH and ΔG values in kcal/mol and ΔS values in cal/(mol·K). Experimental values between brackets.

Equation	NHC	$-\Delta H^0$(298K)	$-\Delta S^0$(298K)	ΔG^0(298K)
S14	IMe	31.4	43.6	−18.4
S14	IMes	27.9 [27.9 ± 1.5]	63.2	−9.0
S14	IPr	13.6; [14.5 ± 1.0]	52.0; [43 ± 3]	1.9
S15	IMe	11.5	27.4	−3.4
S15	IMes	14.1	36.3	−3.3
S15	IPr	12.3	40.1	−0.3
S16	IMe	38.2	68.7	−17.7
S16	IMes	42.4	81.3	−17.9
S16	IPr	38.8; [32.8 ± 1.2]	82.3	−14.2

The superoxide products in reaction S15 were calculated both as triplets and as open-shell singlets, however, the triplet states were found to be thermodynamically more favorable in all cases. Accordingly, the values collected in Table S8 for reaction S15 correspond to the formation of the more stable triplet products. Thermochemical values 2.5, 3.5 and 3.7 kcal/mol less negative in enthalpy and 3.8, 5.8 and 5.2 kcal/mol in Gibbs energy would be obtained for the T-shaped minima in the singlet state when NHC = IMe, IMes and IPr respectively.
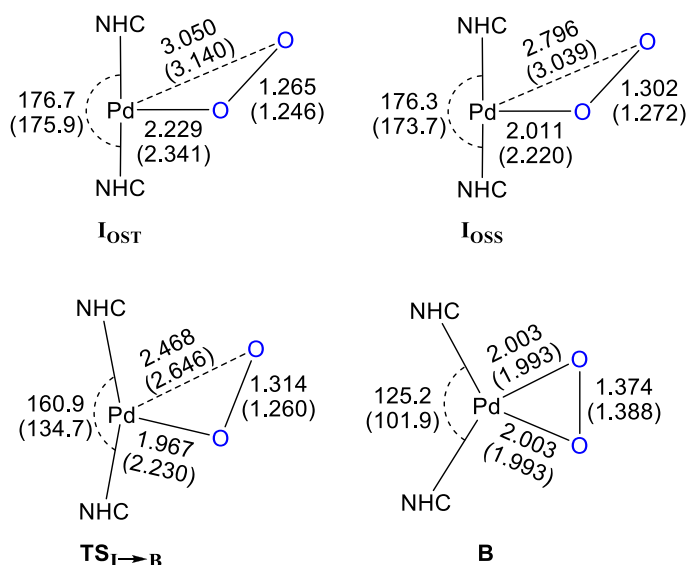
Figure S28. Selected structural parameters (bond lengths in Å and angles in degrees) of all species involved in the first addition of O_2 to [Pd(IPr)$_2$]. For comparison purposes, metrical parameters for the optimized structures for the reaction of the analogous complex with IMe ligands, [Pd(IMe)$_2$], are reported between parentheses.
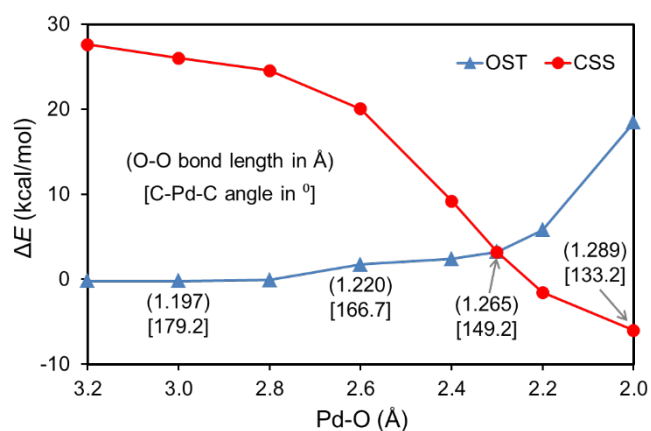
Figure S29. Energy profile for binding of O_2 to $[Pd(IPr)_2]$ by a side-on concerted approach. Energy of the optimized structures at each fixed Pd-O distance (both Pd-O bond distances constrained to be equal) in the triplet state (OST, blue triangles) and energy of those fixed structures as closed-shell singlets (CSS, red circles). OSS data are not shown in the diagram since at low Pd-O bond lengths (≤ 2.3 Å) converge to the CSS and at high Pd-O they reflect essentially the O_2 singlet-triplet gap.
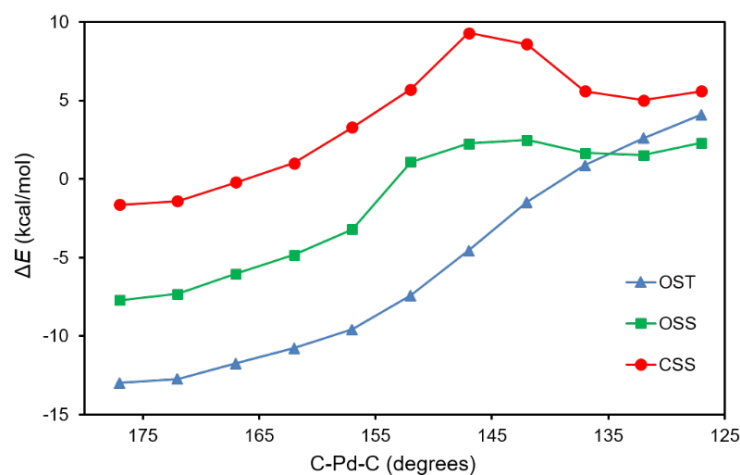
Figure S30. Computed change in energy with the C-Pd-C angle at the BP86-D3(BJ)(PCM)/BSII//PBE0-D3(BJ)/BSI level for $[Pd(IPr)_2(\eta^1\text{-}O_2)]$. At each fixed C-Pd-C angle, the minimum energy structure was computed in the triplet state (OST, blue triangles). Moreover, the energy of those fixed structures were also calculated as closed-shell singlets (CSS, red circles) and open-shell singlets (OSS, green squares).

Table S9. Reaction coordinates and energies of the OST, OSS and CSS states for all the data employed to construct the approximate PES for first O_2 addition to [Pd(IPr)$_2$]. Angles in degrees, distances in Å and energies in kcal/mol.

NHC–Pd–NHC Angle	Pd–O$_2$ Centroid Distance	Tilt Angle	E_{OST}	E_{OSS}	E_{CSS}
117	2.203	4.6	8.4	1.2	1.2
117	2.239	14.0	9.3	4.6	4.6
117	2.298	22.9	7.8	4.6	7.5
122	2.216	4.6	6.9	0.5	0.5
122	2.247	14.0	7.2	3.4	3.4
122	2.305	22.9	5.7	6.2	6.2
127	2.219	0.4	5.6	0.7	0.7
127	2.225	4.5	5.9	1.1	1.1
127	2.258	13.9	5.3	2.8	2.8
127	2.314	22.8	4.1	2.3	5.6
132	2.237	5.7	3.8	1.1	1.1
132	2.271	13.7	3.6	-0.6	2.7
132	2.322	22.7	2.6	1.5	5.0
133	1.893	0.0	18.4	-6.0	-6.0
137	2.258	1.1	3.2	2.5	2.5
137	2.266	6.0	3.0	2.7	2.7
137	2.295	15.4	2.0	3.5	3.5
137	2.347	24.3	0.9	1.7	5.6
142	2.286	2.2	2.6	4.6	4.6
142	2.305	11.8	1.6	0.5	4.5
142	2.346	20.9	-0.3	0.9	5.2
142	2.406	29.6	-1.5	2.5	8.6
145	2.106	0.0	5.8	-1.6	-1.6
147	2.319	0.3	2.2	2.3	6.9
147	2.323	5.2	1.8	2.4	7.0
147	2.331	10.1	1.0	2.0	6.6
147	2.344	14.7	0.0	1.7	6.3
147	2.365	19.3	-1.3	1.4	6.3
147	2.417	28.1	-3.4	1.3	7.7
147	2.487	36.6	-4.6	2.2	9.3
152	2.368	12.1	-0.4	2.7	8.2
152	2.390	21.4	-3.9	5.0	6.9
152	2.446	30.1	-6.3	-0.6	5.4
152	2.515	38.6	-7.4	1.1	5.7
155	2.317	0.0	2.4	4.2	9.2
157	2.516	1.9	1.4	9.8	7.3
157	2.396	17.3	-4.2	1.2	5.5
157	2.464	30.6	-8.3	-2.6	3.3
157	2.534	39.1	-9.6	-3.2	3.3
162	2.426	22.0	-7.1	-1.8	4.1
162	2.478	30.8	-9.8	-4.4	0.8
162	2.550	39.2	-10.8	-4.8	1.0
167	2.527	0.0	1.7	11.3	20.1

167	3.473	3.3	1.6	17.0	47.9
167	2.474	17.2	-5.4	0.8	8.2
167	2.449	22.1	-8.7	-3.3	3.0
167	2.499	30.8	-10.4	-5.0	2.0
167	2.557	39.4	-11.8	-6.0	-0.2
172	3.277	9.0	-1.3	12.8	23.9
172	2.522	30.9	-11.5	-6.1	0.5
172	2.572	39.5	-12.7	-7.3	-1.4
177	3.575	3.4	-1.2	13.0	26.1
177	3.430	8.7	-2.2	11.6	24.2
177	2.477	17.6	-7.1	-0.8	5.9
177	2.489	22.2	-8.9	-3.5	3.2
177	2.550	31.0	-11.7	-6.3	0.3
177	2.597	39.6	-13.0	-7.7	-1.6
178	2.734	0.0	-0.1	12.3	24.6
179	3.347	0.0	1.8	17.0	31.1
179	2.940	0.0	-0.2	14.4	26.0
179	3.144	0.0	-0.2	13.6	27.6

Time Dependent DFT calculations (TD-DFT) were performed to predict the intensity and position of bands in the UV-Vis spectra of the possible intermediate complex $[Pd(IPr)_2(\eta^1-O_2)]$ and to further confirm the identity of the diamagnetic product responsible of the bleaching of $[Pd(IPr)_2]$ solutions when O_2 is added at low temperatures. To reduce the computational cost of the calculations, the arene substituents on the nitrogens of the IPr ligands on the optimized structures were replaced by methyl groups without modification of the rest of the structure. Since the arene substituents in the IPr ligands are essentially perpendicular to the NHC rings, it should be expected that this truncation would not significantly affect the electronic transitions computed. In this way, the UV-Vis spectra of $[Pd(IPr)_2]$, cis-$[Pd(IPr)_2(\eta^2-O_2)]$, and $[Pd(IPr)_2(\eta^1-O_2)]$ were simulated. The computed visible spectra of $[Pd(IPr)_2]$, λ_{max}=470 nm, is in perfect agreement to the experimentally measured one, λ_{max}=473 nm. Bleaching of the product upon reaction with O_2 to form cis-$[Pd(IPr)_2(\eta^2-O_2)]$ is also modeled well by our computed spectrum for "$[Pd(IMe)_2(\eta^2-O_2)]$" in which we have forced a C-Pd-C angle of 125.2 rather than 101.9 °

(see Figure S26). These observations give confidence that the UV-Vis spectra can be modeled by TD-DFT calculations. Moreover, $[Pd(IPr)_2(\eta^1-O_2)]$ is predicted to have an intense broad band with a maximum near 550 nm which extends into the near IR. An absorption matching this was not seen in the kinetic data.

Broken Symmetry Calculations. DFT single-point energy calculations on the electronic structure of a truncated form of *trans*-$[Pd(IPr)_2(\eta^1-O_2)_2]$ were performed with the ORCA electronic structure package[17] at the B3LYP[13] level of theory. The truncation was performed by replacing the ligand ^{i}Pr groups with hydrogens at a C–H distance of 0.95 Å. The calculations were performed using def2- variants of the all-electron Gaussian basis sets of split-valence (def2-SVP; C, H) and triple-valence (def2-TZVP; O, N, Pd-bound C) quality as developed by the Ahlrichs group.[10] The def2-SD effective core potential[11] and corresponding def2-TZVP/def2-TZVP/J basis sets (*ibid*.) were applied to Pd. The calculations employed the resolution of identity (RI-J) algorithm for the computation of the Coulomb terms and the "chain of spheres exchange" (COSX) algorithm for the calculation of the exchange terms.[18] For the fitting basis in the RI-J treatment, the 'def2' fit bases were used.[19] The SCF calculations were tightly converged (1×10^{-8} E_h in energy, 1×10^{-7} E_h in the density change, and 5×10^{-7} in the maximum element of the DIIS error vector). We have used the general abbreviation BS(m,n) to denote a BS-DFT calculation with m unpaired or partially paired spin-up electrons and n partially paired spin-down electrons as the two interacting fragments.[20]

The exchange coupling was treated using the Heisenberg-Dirac-van Vleck (HDvV) Hamiltonian:

$$H_{\text{HDvV}} = -2J\hat{S}_A \bullet \hat{S}_B \tag{S17}$$

For predicting the exchange coupling constant J we have employed the broken symmetry DFT method of Noodleman,[21] which allows one to treat systems with unpaired electrons within the restriction of a single spin-unrestricted determinant. Having obtained spin-unrestricted solutions for the determinants of maximum spin, using $M_S = S_A + S_B$, and broken symmetry spin, using $M_S = |S_A - S_B|$, the following definitions of J were employed.

Noodleman's equation, which is valid in the weak coupling limit, reads:[22]

$$J_1 = -\frac{E_{HS} - E_{BS}}{(S_A + S_B)^2} \tag{S18}$$

where E_{HS} and E_{BS} are the energies of the high-spin (HS) and broken-symmetry (BS) determinants, respectively. The following definition of J given by Bencini[23] is suitable in the strong coupling limit:

$$J_2 = -\frac{E_{HS} - E_{BS}}{(S_A + S_B)(S_A + S_B + 1)} \tag{S19}$$

We have also used an expression for J which is valid over the whole coupling strength regime, as discussed by Yamaguchi and coworkers:[24]

$$J_3 = -\frac{E_{HS} - E_{BS}}{\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{BS}} \tag{S20}$$

Cartesian Coordinates (Unless stated otherwise optimized at the PBE0-D3(BJ)/BSI level)

With empirical dispersion corrections			Without empirical dispersion corrections		
O$_2$ (OST)			**O$_2$ (OST)** at PBE0/BSI level		
8 0.000000	0.000000	0.596497	8 0.000000	0.000000	0.596497
8 0.000000	0.000000	-0.596497	8 0.000000	0.000000	-0.596497
[Pd(IMe)$_2$] (CSS)			**Pd(IMe)$_2$(^{1}-O$_2$)] (OST)**		
46 0.000001	0.000063	-0.000152	46 0.046824	-0.176467	0.139315
6 -2.013401	0.000033	-0.000087	8 0.080728	1.692084	-1.269974
7 -2.861164	0.755844	0.753057	8 -0.995465	2.126227	-1.723177
6 -4.183250	0.478949	0.477513	6 -1.984109	-0.292873	0.204189
1 -4.999970	0.977055	0.973973	7 -2.834942	-0.447178	-0.841364
6 -4.183350	-0.479209	-0.476944	6 -4.151724	-0.370417	-0.444337
1 -5.000160	-0.977487	-0.973087	1 -4.973916	-0.463847	-1.134590
7 -2.861308	-0.755817	-0.753018	6 -4.139709	-0.171693	0.893415
6 2.013398	-0.000181	-0.000160	1 -4.948577	-0.061705	1.596841
7 2.861104	-0.753263	0.755776	7 -2.813233	-0.129566	1.268274
6 4.183216	-0.477775	0.478938	6 2.081652	-0.177664	0.163066
1 4.999895	-0.974356	0.976990	7 2.912248	0.873005	0.389437
6 4.183383	0.477118	-0.478786	6 4.236506	0.518454	0.247000
1 5.000233	0.973511	-0.976743	1 5.044533	1.217813	0.385995
7 2.861364	0.753102	-0.755594	6 4.250499	-0.794875	-0.075356
6 2.404087	1.720280	-1.725713	1 5.072731	-1.463326	-0.271151
1 1.312523	1.696560	-1.701873	7 2.932945	-1.198570	-0.121246
1 2.756305	2.722262	-1.465931	6 2.490058	-2.536816	-0.437649
1 2.756239	1.457375	-2.726904	1 1.400560	-2.535273	-0.370322
6 2.403490	-1.719996	1.726188	1 2.792330	-2.812160	-1.451263
1 1.311929	-1.696230	1.702003	1 2.902164	-3.256009	0.274923
1 2.755772	-2.722088	1.466913	6 2.447799	2.203888	0.714376
1 2.755318	-1.456706	2.727395	1 1.373330	2.142140	0.884162
6 -2.403937	-1.726041	-1.720054	1 2.948976	2.565748	1.615334
1 -1.312369	-1.702321	-1.696105	1 2.632905	2.888824	-0.115613
1 -2.756272	-2.727177	-1.457179	6 -2.342704	0.081305	2.617341
1 -2.755894	-1.466264	-2.722132	1 -1.254626	-0.000289	2.592426
6 -2.403641	1.726336	1.719749	1 -2.623466	1.076418	2.971810
1 -2.755789	1.467025	2.721877	1 -2.754365	-0.676023	3.289498
1 -1.312082	1.702334	1.695915	6 -2.393217	-0.597808	-2.209646
1 -2.755681	2.727465	1.456459	1 -2.556347	0.326795	-2.765557
			1 -1.321975	-0.801505	-2.182009
			1 -2.919708	-1.429438	-2.683836
[Pd(IMe)$_2$(^{1}-O$_2$)] (OSS)			**[Pd(IMe)$_2$(^{2}-O$_2$)] (CSS)**		
46 0.046187	-0.125080	0.086139	46 0.000017	0.955842	-0.000007
8 -0.059844	1.689479	-1.188999	8 -0.679503	2.824459	0.140298
8 -1.206104	2.122147	-1.530933	8 0.679573	2.824451	-0.140222
6 -1.980337	-0.342259	0.202405	7 -1.692862	-1.470102	0.935930
7 -2.842341	-0.510445	-0.828724	7 -2.765989	-0.120372	-0.329960
6 -4.152306	-0.483656	-0.405586	7 1.692795	-1.470204	-0.935865
1 -4.983687	-0.590822	-1.082602	7 2.766018	-0.120411	0.329876
6 -4.121755	-0.308337	0.935198	6 -1.547532	-0.314402	0.236949
1 -4.919592	-0.238638	1.656014	6 -2.967653	-1.983595	0.804393
7 -2.790155	-0.227530	1.285497	1 -3.283479	-2.888446	1.296952
6 2.092189	-0.093499	0.096122	6 -3.642935	-1.130465	0.001431
7 2.930064	0.962967	0.247168	1 -4.661349	-1.152180	-0.349906
6 4.251683	0.578600	0.183320	6 1.547538	-0.314433	-0.236982
1 5.064545	1.278959	0.282962	6 2.967587	-1.983710	-0.804379

6	4.256184	-0.757878	-0.022547	1	3.283365	-2.888614	-1.296883
1	5.072840	-1.449952	-0.145457	6	3.642935	-1.130512	-0.001546
7	2.934656	-1.146768	-0.072109	1	4.661370	-1.152217	0.349723
6	2.487311	-2.502626	-0.294894	6	-3.091968	1.019758	-1.167898
1	1.397498	-2.496656	-0.236430	1	-2.331238	1.790780	-1.011391
1	2.795461	-2.851298	-1.283781	1	-3.110589	0.726876	-2.220807
1	2.892740	-3.168861	0.470709	1	-4.070212	1.410261	-0.881556
6	2.484849	2.319973	0.494876	6	-0.656592	-2.052011	1.757224
1	1.488785	2.438868	0.069591	1	0.212928	-1.399460	1.696868
1	2.463513	2.526006	1.568194	1	-0.987830	-2.117734	2.796063
1	3.168495	3.016171	0.005774	1	-0.393283	-3.050451	1.397570
6	-2.301677	-0.018486	2.628420	6	3.092050	1.019730	1.167771
1	-1.211803	-0.036427	2.580629	1	2.331395	1.790809	1.011195
1	-2.629703	0.951875	3.009236	1	3.110600	0.726904	2.220694
1	-2.654860	-0.810930	3.293349	1	4.070341	1.410125	0.881452
6	-2.424500	-0.588128	-2.211180	6	0.656445	-2.052172	-1.757021
1	-2.558081	0.379779	-2.696076	1	-0.213096	-1.399652	-1.696563
1	-1.361433	-0.830122	-2.218945	1	0.987552	-2.117896	-2.795906
1	-2.990116	-1.367228	-2.727030	1	0.393224	-3.050619	-1.397319

[Pd(IMe)$_2$(^{1}-O$_2$)$_2$] (OST)   **TS$_{I→B}$ (NHC = IMe, OST)**

8	-0.055705	-2.035062	0.050266	46	0.009041	0.516281	-0.017526
8	-1.108077	-2.594151	-0.455246	8	-0.736120	2.617561	0.012865
6	-2.037371	0.144779	0.064976	8	0.414467	3.129324	0.067209
7	-2.890054	-0.476903	0.906338	6	1.917876	-0.288503	-0.164056
6	-4.199592	-0.211120	0.573485	7	3.067483	0.142988	0.421325
1	-5.030575	-0.616222	1.126399	6	4.129178	-0.690563	0.143533
6	-4.165184	0.612971	-0.497998	1	5.123564	-0.513306	0.519514
1	-4.959426	1.067525	-1.066289	6	3.646594	-1.678438	-0.644622
7	-2.834123	0.824320	-0.787524	1	4.139919	-2.525245	-1.092938
6	2.036992	-0.144383	0.063978	7	2.304312	-1.417389	-0.818471
7	2.832459	-0.825705	-0.788298	6	-1.874022	-0.266811	0.135066
6	4.163939	-0.616834	-0.498732	7	-2.983612	0.010960	-0.601170
1	4.957366	-1.073084	-1.066806	6	-4.062858	-0.755624	-0.213179
6	4.199817	0.207744	0.572325	1	-5.030003	-0.680101	-0.682801
1	5.031552	0.611694	1.124959	6	-3.632815	-1.539249	0.800965
7	2.890780	0.475995	0.905124	1	-4.154221	-2.274166	1.392137
6	2.486938	1.377206	1.963821	7	-2.302544	-1.230652	0.996084
1	1.430600	1.210465	2.166837	6	-1.454477	-1.830888	1.998873
1	3.074577	1.174135	2.860996	1	-0.431468	-1.520970	1.775353
1	2.615975	2.412112	1.643808	1	-1.726531	-1.482989	2.998834
6	2.356120	-1.615652	-1.906370	1	-1.534107	-2.920303	1.957883
1	1.333271	-1.922960	-1.701207	6	-3.014134	0.989411	-1.665222
1	2.395781	-1.030607	-2.828248	1	-2.045295	1.486137	-1.685461
1	2.979991	-2.504734	-2.010200	1	-3.200205	0.504264	-2.627132
6	-2.359003	1.613764	-1.906557	1	-3.791987	1.732196	-1.474113
1	-1.340750	1.932960	-1.696451	6	1.402273	-2.223907	-1.607047
1	-2.386742	1.023861	-2.825759	1	0.398241	-1.830107	-1.436390
1	-2.991964	2.495368	-2.018557	1	1.646928	-2.153000	-2.670102
6	-2.484845	-1.377056	1.965474	1	1.452666	-3.269028	-1.290672
1	-2.610491	-2.412325	1.645217	6	3.147032	1.330920	1.243489
1	-1.429298	-1.207343	2.169980	1	4.033233	1.909169	0.972999
1	-3.074366	-1.175873	2.861827	1	2.253781	1.928280	1.054257
46	-0.000032	0.001037	0.045548	1	3.195466	1.065732	2.303060
8	0.054332	2.037149	0.042702				
8	1.112656	2.596421	-0.449924				

TS [Pd(IMe)₂(²-O₂)] + O₂ (OST)			
46	0.058995	-0.666731	-0.044485
8	0.763057	-3.088325	-0.063657
8	-0.457660	-2.711639	-0.133677
7	2.544775	1.036570	-0.954453
7	3.052026	-0.210442	0.699999
7	-2.510920	0.526644	1.097561
7	-2.860828	-0.356679	-0.815809
6	2.016763	0.106429	-0.118542
6	3.867103	1.294585	-0.663157
1	4.462055	1.997689	-1.222546
6	4.187416	0.504812	0.388065
1	5.114437	0.391181	0.925765
6	-1.875630	-0.128221	0.090720
6	-3.850363	0.708508	0.820538
1	-4.522928	1.202780	1.501890
6	-4.070322	0.154304	-0.392413
1	-4.970545	0.079559	-0.979902
6	2.951507	-1.186789	1.764168
1	2.187349	-1.915195	1.488050
1	3.910348	-1.694758	1.881508
1	2.677230	-0.706046	2.706830
6	1.809195	1.632523	-2.045780
1	0.778784	1.285257	-1.960636
1	1.837394	2.722205	-1.975090
1	2.224288	1.315407	-3.005842
6	-2.642116	-1.035170	-2.074319
1	-2.553094	-0.316096	-2.893439
1	-1.719548	-1.608917	-1.987002
1	-3.472548	-1.714812	-2.275111
6	-1.860956	0.925245	2.324016
1	-0.786180	0.821196	2.166709
1	-2.103143	1.964428	2.557361
1	-2.167594	0.280871	3.151829
8	-0.127598	2.769302	0.202199
8	-1.225428	3.247521	0.147018

[Pd(IMes)₂] (CSS)				**[Pd(IMes)₂] (CSS)** at PBE0/BSI level			
46	-0.000002	0.000058	0.000067	46	0.000682	0.000008	0.000237
7	-1.001259	2.835659	0.364542	7	-0.910823	-2.852467	-0.551747
7	1.001185	2.835253	-0.368000	7	0.912484	-2.850897	0.558566
7	-1.001351	-2.835461	-0.364774	7	-0.911660	2.852527	0.551064
7	1.001083	-2.835243	0.367796	7	0.911637	2.850864	-0.559270
6	0.000042	1.988387	-0.001053	6	0.000717	-2.000545	0.002379
6	-0.634705	4.164958	0.229659	6	-0.575387	-4.180936	-0.346420
1	-1.303193	4.973965	0.473025	1	-1.181952	-4.991781	-0.714965
6	0.634378	4.164689	-0.235310	6	0.577424	-4.179944	0.356421
1	1.302718	4.973422	-0.479972	1	1.184171	-4.989749	0.726970
6	-2.264514	2.380696	0.848765	6	-2.071747	-2.422447	-1.266878
6	-3.246495	2.003778	-0.065806	6	-3.248294	-2.164419	-0.559833
6	-4.480436	1.601561	0.437775	6	-4.374554	-1.786609	-1.285664
1	-5.258638	1.312407	-0.262266	1	-5.297821	-1.584472	-0.748602
6	-4.731289	1.539344	1.803900	6	-4.346574	-1.656039	-2.671920
6	-3.710942	1.890965	2.685542	6	-3.149895	-1.908245	-3.337162
1	-3.882967	1.826023	3.756732	1	-3.107251	-1.800892	-4.417990
6	-2.467614	2.313163	2.228620	6	-1.997552	-2.289012	-2.654838
6	-2.951476	1.955588	-1.531279	6	-3.276787	-2.239593	0.936048

1	-2.212460	1.165608	-1.716106	1	-2.633077	-1.457002	1.353884
1	-2.522347	2.894108	-1.893901	1	-2.902090	-3.199664	1.303227
1	-3.853870	1.733913	-2.103658	1	-4.291432	-2.096037	1.312616
6	-6.056027	1.056734	2.319807	6	-5.569214	-1.217332	-3.426617
1	-5.986642	0.018912	2.665830	1	-5.639284	-0.124049	-3.455018
1	-6.822776	1.095346	1.542703	1	-6.483115	-1.591116	-2.957824
1	-6.399386	1.657196	3.166439	1	-5.548142	-1.570616	-4.460364
6	-1.347618	2.623779	3.173990	6	-0.700451	-2.499245	-3.376213
1	-0.501260	1.957401	2.974897	1	0.043298	-1.777519	-3.020643
1	-1.664419	2.489297	4.209693	1	-0.829096	-2.368637	-4.452459
1	-0.983499	3.648789	3.056179	1	-0.290205	-3.497953	-3.198328
6	2.264654	2.379672	-0.851062	6	2.072685	-2.418686	1.273554
6	3.246368	2.004508	0.064423	6	3.249739	-2.162189	0.567068
6	4.480452	1.601244	-0.438094	6	4.375134	-1.781683	1.293096
1	5.258417	1.313310	0.262695	1	5.298896	-1.580700	0.756479
6	4.731597	1.536319	-1.803975	6	4.345589	-1.647058	2.678798
6	3.711420	1.886252	-2.686580	6	3.148256	-1.898101	3.343599
1	3.883621	1.819038	-3.757610	1	3.104407	-1.787721	4.424089
6	2.468091	2.309470	-2.230781	6	1.996963	-2.281381	2.661198
6	2.951082	1.958943	1.529924	6	3.279855	-2.241550	-0.928563
1	2.520593	2.897607	1.890527	1	2.905123	-3.202471	-1.293459
1	3.853646	1.739638	2.102947	1	4.294978	-2.099526	-1.304437
1	2.213054	1.168368	1.716177	1	2.636969	-1.459848	-1.349351
6	6.056579	1.053332	-2.318949	6	5.566635	-1.204922	3.434059
1	5.984115	0.019991	-2.677402	1	5.620144	-0.111461	3.484003
1	6.819683	1.079622	-1.537776	1	6.482782	-1.555397	2.952031
1	6.406922	1.661977	-3.156907	1	5.557918	-1.578802	4.460787
6	1.348280	2.618228	-3.176986	6	0.699127	-2.490399	3.381590
1	1.665283	2.481678	-4.212358	1	0.826293	-2.356393	4.457594
1	0.984186	3.643481	-3.061289	1	0.289902	-3.489968	3.206181
1	0.501857	1.952295	-2.976747	1	-0.044676	-1.770321	3.022797
6	-0.000036	-1.988282	0.001012	6	0.000180	2.000557	-0.002512
6	-0.634820	-4.164794	-0.230144	6	-0.576659	4.180987	0.344901
1	-1.303318	-4.973739	-0.473697	1	-1.183505	4.991861	0.712937
6	0.634237	-4.164645	0.234892	6	0.576123	4.179922	-0.357986
1	1.302557	-4.973436	0.479405	1	1.182571	4.989695	-0.729081
6	-2.264637	-2.380454	-0.848874	6	-2.072374	2.422523	1.266555
6	-3.246725	-2.004012	0.065803	6	-3.248830	2.163609	0.559864
6	-4.480728	-1.601939	-0.437665	6	-4.374874	1.785650	1.286145
1	-5.259022	-1.313249	0.262461	1	-5.298137	1.582828	0.749356
6	-4.731577	-1.539356	-1.803794	6	-4.346615	1.655816	2.672364
6	-3.711148	-1.890453	-2.685518	6	-3.149905	1.909054	3.337359
1	-3.883190	-1.825273	-3.756692	1	-3.107055	1.802381	4.418256
6	-2.467713	-2.312532	-2.228696	6	-1.997933	2.289965	2.654687
6	-2.951799	-1.956397	1.531307	6	-3.277672	2.237946	-0.936047
1	-2.522529	-2.895000	1.893542	1	-2.902873	3.197731	-1.303861
1	-3.854269	-1.735128	2.103717	1	-4.292442	2.094396	-1.312284
1	-2.212921	-1.166375	1.716531	1	-2.634235	1.454988	-1.353626
6	-6.056382	-1.056715	-2.319487	6	-5.568539	1.216528	3.427871
1	-6.824364	-1.100706	-1.543877	1	-6.483844	1.571976	2.947838
1	-6.397137	-1.653478	-3.169755	1	-5.557136	1.587628	4.455562
1	-5.988419	-0.016979	-2.660039	1	-5.626457	0.123167	3.474881
6	-1.347636	-2.622606	-3.174155	6	-0.700816	2.501432	3.375676
1	-0.501414	-1.956136	-2.974819	1	0.043389	1.780124	3.020217
1	-1.664448	-2.487824	-4.209818	1	-0.829115	2.371155	4.452004
1	-0.983310	-3.647586	-3.056700	1	-0.291365	3.500383	3.197292

6	2.264535	-2.379775	0.851002	6	2.072055	2.418631	-1.273884
6	2.467922	-2.309854	2.230737	6	1.996529	2.280259	-2.661368
6	3.711247	-1.886751	2.686667	6	3.148148	1.897102	-3.343405
1	3.883418	-1.819782	3.757714	1	3.104462	1.785898	-4.423806
6	4.731455	-1.536638	1.804177	6	4.345521	1.647248	-2.678363
6	4.480365	-1.601290	0.438265	6	4.374855	1.782827	-1.292688
1	5.258362	-1.313240	-0.262448	1	5.298672	1.582706	-0.755826
6	3.246302	-2.004461	-0.064378	6	3.249224	2.163215	-0.567080
6	1.348068	-2.618752	3.176844	6	0.698657	2.487917	-3.382084
1	1.665011	-2.482316	4.212249	1	0.826105	2.353445	-4.457994
1	0.983993	-3.643997	3.061015	1	0.288630	3.487257	-3.207271
1	0.501639	-1.952806	2.976640	1	-0.044654	1.767454	-3.023038
6	6.056400	-1.053665	2.319250	6	5.567128	1.205501	-3.432951
1	6.405674	-1.660995	3.158596	1	5.552279	1.568026	-4.463639
1	5.984403	-0.019596	2.675714	1	5.628409	0.111974	-3.470962
1	6.820068	-1.081916	1.538693	1	6.482396	1.567770	-2.957939
6	2.951112	-1.958744	-1.529897	6	3.279090	2.243623	0.928506
1	2.520614	-2.897368	-1.890597	1	2.904257	3.204785	1.292674
1	3.853724	-1.739431	-2.102842	1	4.294153	2.101888	1.304653
1	2.213113	-1.168150	-1.716141	1	2.636152	1.462187	1.349706

[Pd(IMes)$_2$(^{1}-O$_2$)] (OST)				[Pd(IMes)$_2$(^{1}-O$_2$)] (OSS)			
46	-0.002637	-0.022018	0.007497	46	-0.005018	0.030181	0.006947
8	-0.175149	0.067156	-2.237175	8	0.304963	0.017664	-1.998659
8	0.522868	0.918760	-2.854975	8	-0.461886	-0.830759	-2.624634
6	-0.007393	1.976671	0.308469	6	0.009696	-1.997837	0.214997
7	-1.014854	2.863359	0.096798	7	1.029407	-2.859362	-0.012629
6	-0.637768	4.156648	0.418144	6	0.642523	-4.172340	0.192793
1	-1.312280	4.990842	0.321915	1	1.322991	-4.996042	0.056794
6	0.643199	4.088079	0.841259	6	-0.656027	-4.136587	0.565423
1	1.322862	4.849266	1.185986	1	-1.348144	-4.921450	0.820444
7	1.007061	2.754002	0.765251	7	-1.020556	-2.800757	0.574633
6	-2.302724	2.497813	-0.402449	6	2.345483	-2.458346	-0.404306
6	-2.615446	2.796374	-1.732041	6	2.717919	-2.596485	-1.743953
6	-3.875665	2.438390	-2.197967	6	4.011759	-2.221094	-2.091824
1	-4.128625	2.650312	-3.233263	1	4.318626	-2.314459	-3.130088
6	-4.809854	1.810223	-1.377644	6	4.911743	-1.723195	-1.152862
6	-4.459426	1.538961	-0.060532	6	4.494542	-1.595090	0.166827
1	-5.175497	1.051424	0.593105	1	5.180914	-1.201289	0.909855
6	-3.204439	1.859660	0.449252	6	3.207842	-1.947900	0.564517
6	2.287336	2.243174	1.138566	6	-2.309182	-2.311148	0.949617
6	2.475509	1.805444	2.450967	6	-2.524434	-1.964538	2.284879
6	3.735661	1.338730	2.806643	6	-3.787695	-1.508678	2.644112
1	3.897979	0.987225	3.822231	1	-3.972139	-1.230894	3.678571
6	4.785151	1.303695	1.890420	6	-4.815103	-1.401698	1.708749
6	4.546225	1.725186	0.587226	6	-4.548544	-1.731884	0.384842
1	5.347167	1.675574	-0.144756	1	-5.331967	-1.624555	-0.359296
6	3.298093	2.190261	0.180621	6	-3.294659	-2.177346	-0.027092
6	0.004371	-2.039857	-0.069926	6	-0.017003	2.044909	-0.034980
7	1.015960	-2.845209	-0.485254	7	-1.049796	2.841646	-0.398116
6	0.644125	-4.178356	-0.492165	6	-0.683689	4.175706	-0.411250
1	1.321065	-4.960945	-0.791467	1	-1.376096	4.955814	-0.679933
6	-0.638931	-4.219337	-0.069844	6	0.616793	4.219991	-0.043467
1	-1.317573	-5.043654	0.072344	1	1.297658	5.046147	0.074937
7	-1.008293	-2.907716	0.181309	7	1.002840	2.909316	0.181390
6	2.297002	-2.348932	-0.878914	6	-2.347006	2.346191	-0.744320
6	3.220306	-2.012453	0.109583	6	-3.268747	2.104973	0.272687

6	4.460144	-1.530725	-0.299283	6	-4.532143	1.649787	-0.093046
1	5.192161	-1.267536	0.457407	1	-5.265313	1.460409	0.684829
6	4.772099	-1.359094	-1.642784	6	-4.866155	1.413206	-1.421648
6	3.816500	-1.697825	-2.598167	6	-3.904908	1.641328	-2.403362
1	4.039439	-1.557016	-3.652178	1	-4.142274	1.437182	-3.443705
6	2.570192	-2.199143	-2.240565	6	-2.634762	2.112041	-2.091087
6	-2.294605	-2.504563	0.651835	6	2.307290	2.503139	0.600546
6	-3.253072	-2.083492	-0.268749	6	3.242893	2.127780	-0.361591
6	-4.512753	-1.748811	0.221716	6	4.512616	1.768622	0.084712
1	-5.274914	-1.427120	-0.481941	1	5.257045	1.473210	-0.648379
6	-4.811777	-1.797653	1.578802	6	4.842336	1.754065	1.434751
6	-3.813349	-2.190147	2.468065	6	3.863091	2.097093	2.365436
1	-4.024052	-2.213850	3.533927	1	4.096008	2.064069	3.426456
6	-2.544919	-2.547386	2.024903	6	2.586183	2.475867	1.968575
6	2.869851	-2.106900	1.562241	6	-2.894281	2.266166	1.714447
1	2.160051	-1.311827	1.817570	1	-2.215873	1.459152	2.013462
1	2.394506	-3.061088	1.806432	1	-2.378972	3.212072	1.902480
1	3.758752	-1.987258	2.184100	1	-3.779044	2.218061	2.351748
6	1.536791	-2.530079	-3.273544	6	-1.590825	2.314477	-3.143238
1	1.284620	-3.595348	-3.267819	1	-1.241112	3.351936	-3.168323
1	0.619116	-1.967324	-3.082701	1	-0.732552	1.668891	-2.929031
1	1.895227	-2.269689	-4.270475	1	-1.983038	2.058119	-4.127986
6	6.094999	-0.784135	-2.057404	6	-6.227405	0.904377	-1.796913
1	6.537420	-1.349678	-2.882077	1	-6.741758	1.602423	-2.464660
1	5.977944	0.250028	-2.399991	1	-6.156751	-0.052884	-2.323463
1	6.805402	-0.782149	-1.227559	1	-6.855684	0.760225	-0.915123
6	1.331007	1.788153	3.417389	6	-1.407536	-2.037912	3.282011
1	0.873204	2.776250	3.523041	1	-0.961263	-3.035990	3.319519
1	0.549692	1.110493	3.054833	1	-0.606708	-1.342468	3.007433
1	1.658202	1.452003	4.402809	1	-1.761772	-1.780870	4.281730
6	3.028960	2.569043	-1.242071	6	-2.994576	-2.449346	-1.467322
1	2.272152	1.908712	-1.681408	1	-2.259466	-1.729809	-1.851296
1	2.645332	3.590958	-1.322537	1	-2.565994	-3.445841	-1.609998
1	3.940924	2.497507	-1.837616	1	-3.902900	-2.375140	-2.068266
6	6.140884	0.809959	2.304745	6	-6.179431	-0.938064	2.128938
1	6.796506	0.678553	1.440976	1	-6.810100	-0.723931	1.263440
1	6.626834	1.516200	2.985893	1	-6.686607	-1.701579	2.728031
1	6.071819	-0.148342	2.828862	1	-6.120813	-0.033233	2.741530
6	-2.828849	1.479013	1.847351	6	2.754392	-1.730979	1.975354
1	-2.300971	2.286079	2.362578	1	2.242618	-2.608933	2.379811
1	-3.713372	1.207383	2.426246	1	3.600473	-1.487639	2.620464
1	-2.153364	0.615018	1.819012	1	2.044883	-0.895838	2.007681
6	-1.611451	3.444873	-2.635934	6	1.741207	-3.080083	-2.768311
1	-2.009819	3.530752	-3.648187	1	2.210646	-3.121772	-3.753051
1	-1.341601	4.448115	-2.291820	1	1.364733	-4.080024	-2.529400
1	-0.693795	2.851151	-2.678391	1	0.875728	-2.400046	-2.812331
6	-6.149691	1.399865	-1.915453	6	6.291762	-1.302279	-1.567929
1	-6.589002	2.182691	-2.539524	1	6.761123	-2.050806	-2.212233
1	-6.059850	0.501961	-2.537345	1	6.260640	-0.364148	-2.133587
1	-6.850038	1.175629	-1.107563	1	6.938668	-1.148133	-0.701132
6	-2.923821	-1.942305	-1.721769	6	2.878167	2.047867	-1.810866
1	-3.827874	-1.760812	-2.305710	1	3.772035	1.931004	-2.426200
1	-2.239146	-1.100934	-1.874492	1	2.222122	1.187465	-1.986357
1	-2.427303	-2.833846	-2.115044	1	2.338324	2.937860	-2.145498
6	-1.454838	-2.917740	2.984508	6	1.517173	2.793931	2.970114
1	-1.066319	-3.922586	2.793694	1	1.105627	3.796926	2.823515

1	-0.612796	-2.225057	2.881615
1	-1.814492	-2.879458	4.014079
6	-6.166238	-1.390140	2.081205
1	-6.514372	-2.053831	2.876957
1	-6.141633	-0.374917	2.494414
1	-6.907600	-1.402255	1.279191

1	0.683662	2.090361	2.870704
1	1.906428	2.728688	3.987419
6	6.221136	1.369828	1.886742
1	6.759529	2.235177	2.286932
1	6.184084	0.617022	2.680176
1	6.810111	0.965007	1.060997

[Pd(IMes)$_2$(^{2}-O$_2$)] (CSS)   **[Pd(IMes)$_2$(^{2}-O$_2$)] (CSS)** at PBE0/BSI level

46	-0.000133	-0.000024	-1.035377
8	0.106603	0.683132	-2.915827
8	-0.107026	-0.683072	-2.915874
7	1.100749	2.406250	0.577124
7	-1.008193	2.498805	0.258161
7	-1.100648	-2.406234	0.577440
7	1.008289	-2.498635	0.258421
6	0.057981	1.665385	0.109684
6	0.690307	3.664919	0.991268
1	1.389421	4.390918	1.370420
6	-0.640246	3.720831	0.791395
1	-1.358688	4.504960	0.961556
6	2.476814	2.029781	0.665702
6	3.010344	1.828596	1.942248
6	4.383120	1.645618	2.058066
1	4.812174	1.500168	3.046410
6	5.216315	1.659324	0.942156
6	4.641672	1.833291	-0.311255
1	5.278245	1.847745	-1.191365
6	3.272293	2.032724	-0.482363
6	2.134543	1.840428	3.161518
1	2.629171	1.334708	3.992935
1	1.179088	1.345460	2.971504
1	1.905159	2.861624	3.483283
6	6.697848	1.482031	1.099730
1	6.945477	0.452957	1.381037
1	7.092813	2.136497	1.881763
1	7.226428	1.705640	0.170991
6	2.700120	2.298156	-1.838520
1	2.066314	1.477887	-2.197281
1	3.500890	2.458768	-2.562615
1	2.063518	3.188466	-1.827186
6	-2.363734	2.200305	-0.088292
6	-2.815479	2.460194	-1.382732
6	-4.162634	2.219995	-1.647034
1	-4.534049	2.408101	-2.650495
6	-5.040532	1.770965	-0.667656
6	-4.551069	1.554185	0.617912
1	-5.223529	1.219102	1.400979
6	-3.212615	1.757431	0.927398
6	-1.905152	2.968204	-2.453532
1	-1.215460	3.725668	-2.070791
1	-2.484184	3.407983	-3.268084
1	-1.296328	2.143331	-2.851777
6	-6.479313	1.505241	-0.997924
1	-6.817708	2.126730	-1.830073
1	-7.130076	1.696678	-0.141014
1	-6.620057	0.458796	-1.289768
6	-2.686355	1.532138	2.312096

46	0.000038	0.000086	-0.985277
8	0.052735	0.687870	-2.868421
8	-0.052777	-0.687571	-2.868469
7	0.979659	2.488922	0.592034
7	-1.132966	2.512987	0.266908
7	-0.979677	-2.488927	0.591682
7	1.132952	-2.512951	0.266616
6	-0.040123	1.705408	0.135937
6	0.531189	3.740635	0.983100
1	1.205620	4.495249	1.351849
6	-0.798981	3.753705	0.779784
1	-1.538690	4.521128	0.936185
6	2.374490	2.172654	0.666464
6	2.929317	1.958432	1.932004
6	4.310691	1.821523	2.028765
1	4.755206	1.668815	3.009210
6	5.132244	1.895165	0.907206
6	4.538633	2.094440	-0.335038
1	5.165792	2.163259	-1.219703
6	3.161550	2.248789	-0.487452
6	2.070590	1.911967	3.163603
1	2.612089	1.450770	3.991977
1	1.152299	1.345279	2.990175
1	1.769110	2.915422	3.482904
6	6.621580	1.756059	1.038231
1	6.921357	0.702380	1.031732
1	6.981384	2.192807	1.973455
1	7.140581	2.247439	0.211908
6	2.568798	2.536903	-1.832229
1	1.939060	1.715927	-2.198044
1	3.359435	2.717472	-2.563164
1	1.929489	3.425118	-1.796561
6	-2.488510	2.208180	-0.089130
6	-2.934894	2.477377	-1.386235
6	-4.285935	2.265127	-1.655059
1	-4.650059	2.466678	-2.658864
6	-5.176702	1.825034	-0.682332
6	-4.693461	1.593268	0.602793
1	-5.374517	1.264458	1.382587
6	-3.352877	1.780554	0.921688
6	-2.016987	2.973007	-2.458602
1	-1.346154	3.753727	-2.088398
1	-2.592541	3.382297	-3.291563
1	-1.390127	2.149969	-2.830022
6	-6.621144	1.591333	-1.018914
1	-6.955635	2.255741	-1.819354
1	-7.266595	1.752310	-0.151443
1	-6.778221	0.562306	-1.361292
6	-2.850304	1.557509	2.317062

1	-2.360984	2.468985	2.776443	1	-2.545285	2.497670	2.789381
1	-1.821010	0.865334	2.290121	1	-1.978418	0.898989	2.315173
1	-3.451547	1.082765	2.946118	1	-3.624402	1.101875	2.936532
6	-0.057974	-1.665357	0.109811	6	0.040108	-1.705348	0.135740
6	-0.690074	-3.664788	0.991799	6	-0.531224	-3.740686	0.982569
1	-1.389108	-4.390795	1.371087	1	-1.205661	-4.495332	1.351188
6	0.640485	-3.720589	0.791928	6	0.798945	-3.753764	0.779274
1	1.359012	-4.504612	0.962221	1	1.538648	-4.521235	0.935568
6	-2.476753	-2.029890	0.665846	6	-2.374499	-2.172701	0.666189
6	-3.272100	-2.033111	-0.482294	6	-3.161611	-2.248585	-0.487702
6	-4.641510	-1.833636	-0.311378	6	-4.538694	-2.094354	-0.335193
1	-5.277987	-1.848267	-1.191555	1	-5.165892	-2.162988	-1.219848
6	-5.216274	-1.659366	0.941924	6	-5.132271	-1.895438	0.907126
6	-4.383194	-1.645414	2.057931	6	-4.310662	-1.822041	2.028663
1	-4.812353	-1.499700	3.046191	1	-4.755141	-1.669632	3.009179
6	-3.010422	-1.828444	1.942306	6	-2.929286	-1.958833	1.931792
6	-2.699756	-2.298788	-1.838334	6	-2.568962	-2.536332	-1.832599
1	-3.500423	-2.459982	-2.562416	1	-3.359658	-2.716842	-2.563480
1	-2.062779	-3.188820	-1.826659	1	-1.929549	-3.424468	-1.797197
1	-2.066277	-1.478360	-2.197329	1	-1.939392	-1.715202	-2.198315
6	-6.697846	-1.482269	1.099383	6	-6.621615	-1.756456	1.038259
1	-6.945442	-0.454001	1.383656	1	-6.921461	-0.702790	1.031952
1	-7.093226	-2.139003	1.879311	1	-6.981340	-2.193385	1.973434
1	-7.226082	-1.703056	0.169781	1	-7.140631	-2.247732	0.211879
6	-2.134753	-1.840056	3.161672	6	-2.070538	-1.912666	3.163385
1	-1.905423	-2.861202	3.483638	1	-1.769000	-2.916187	3.482398
1	-2.629470	-1.334190	3.992946	1	-2.612049	-1.451736	3.991901
1	-1.179267	-1.345135	2.971685	1	-1.152287	-1.345883	2.990105
6	2.363774	-2.200129	-0.088231	6	2.488521	-2.208100	-0.089358
6	2.815309	-2.460010	-1.382745	6	2.934907	-2.477061	-1.386520
6	4.162436	-2.219888	-1.647241	6	4.285969	-2.264838	-1.655274
1	4.533691	-2.408005	-2.650759	1	4.650095	-2.466204	-2.659113
6	5.040523	-1.770980	-0.667975	6	5.176743	-1.824986	-0.682448
6	4.551264	-1.554201	0.617667	6	4.693508	-1.593445	0.602716
1	5.223853	-1.219208	1.400661	1	5.374567	-1.264818	1.382574
6	3.212835	-1.757331	0.927340	6	3.352907	-1.780715	0.921564
6	1.904809	-2.968012	-2.453404	6	2.016973	-2.972400	-2.459001
1	1.215057	-3.725338	-2.070503	1	1.346052	-3.753122	-2.088958
1	2.483705	-3.407967	-3.267959	1	2.592508	-3.381588	-3.292025
1	1.296027	-2.143131	-2.851696	1	1.390214	-2.149228	-2.830284
6	6.479289	-1.505420	-0.998448	6	6.621192	-1.591286	-1.018968
1	6.817525	-2.127066	-1.830545	1	6.955623	-2.255455	-1.819629
1	7.130139	-1.696814	-0.141595	1	7.266639	-1.752592	-0.151561
1	6.620119	-0.459032	-1.290467	1	6.778339	-0.562163	-1.361008
6	2.686811	-1.532005	2.312125	6	2.850311	-1.557898	2.316969
1	3.452095	-1.082549	2.945978	1	3.624409	-1.102388	2.936528
1	2.361587	-2.468847	2.776587	1	2.545259	-2.498138	2.789122
1	1.821422	-0.865250	2.290282	1	1.978437	-0.899351	2.315175
[Pd(IMes)$_2$(^{2}-O$_2$)], X-ray constrained (CSS)				**[Pd(IMes)$_2$(^{1}-O$_2$)$_2$] (OST)**			
46	-0.000045	0.000036	-1.045223	46	-0.005576	0.000015	-0.000022
8	0.149219	0.705930	-2.920688	8	0.138811	0.097886	2.018226
8	-0.149475	-0.705818	-2.920807	8	-0.740037	0.793675	2.661202
7	1.137807	2.387378	0.572902	8	0.138273	-0.097602	-2.018300
7	-0.970993	2.493763	0.252907	8	-0.740311	-0.793843	-2.661135
7	-1.137767	-2.387304	0.573038	6	-0.021698	-2.025106	0.150319
7	0.971016	-2.493650	0.252949	7	0.935982	-2.894166	-0.236877

6	0.090018	1.653465	0.106256		6	0.564409	-4.200674	0.032845
6	0.734998	3.649414	0.984556		1	1.205521	-5.034921	-0.196820
1	1.438867	4.371212	1.362829		6	-0.661357	-4.140544	0.599635
6	-0.595003	3.713905	0.784061		1	-1.320870	-4.912667	0.958478
1	-1.308431	4.502915	0.952642		7	-1.000235	-2.800901	0.665030
6	2.511855	2.004075	0.666954		6	2.203336	-2.496694	-0.770280
6	3.040806	1.809612	1.946621		6	2.444524	-2.650106	-2.137902
6	4.412339	1.621182	2.067810		6	3.687275	-2.250987	-2.620557
1	4.837623	1.479816	3.058372		1	3.889601	-2.353040	-3.683099
6	5.249117	1.624919	0.954512		6	4.667582	-1.725301	-1.783646
6	4.679169	1.794613	-0.301525		6	4.389576	-1.609652	-0.426246
1	5.318477	1.802554	-1.179724		1	5.147967	-1.218783	0.244944
6	3.311031	1.997426	-0.478569		6	3.157663	-1.977157	0.106966
6	2.162812	1.835155	3.164194		6	-2.200677	-2.284527	1.253157
1	2.648563	1.322856	3.996839		6	-2.235960	-2.105869	2.638099
1	1.200313	1.354473	2.973590		6	-3.392639	-1.567950	3.189093
1	1.948690	2.859963	3.485033		1	-3.429587	-1.399168	4.261387
6	6.729012	1.439515	1.117556		6	-4.487684	-1.223649	2.400648
1	6.969094	0.409693	1.402881		6	-4.416567	-1.443215	1.029676
1	7.125409	2.093925	1.898885		1	-5.267006	-1.193446	0.402505
1	7.261978	1.656787	0.189829		6	-3.276916	-1.968563	0.425026
6	2.745282	2.254902	-1.838688		6	-0.021625	2.025147	-0.150315
1	2.122657	1.427290	-2.200333		7	-1.000090	2.800993	-0.665062
1	3.549247	2.422784	-2.557587		6	-0.661169	4.140630	-0.599590
1	2.098506	3.137761	-1.833861		1	-1.320653	4.912787	-0.958417
6	-2.329054	2.203208	-0.091883		6	0.564577	4.200685	-0.032746
6	-2.781997	2.468095	-1.385013		1	1.205732	5.034886	0.196971
6	-4.131271	2.236051	-1.646203		7	0.936083	2.894148	0.236964
1	-4.503817	2.427508	-2.648583		6	-2.200573	2.284668	-1.253155
6	-5.009758	1.791830	-0.665157		6	-3.276709	1.968568	-0.424975
6	-4.518920	1.571044	0.619228		6	-4.416373	1.443145	-1.029576
1	-5.191866	1.240053	1.403555		1	-5.266717	1.193208	-0.402348
6	-3.178467	1.765242	0.925585		6	-4.487581	1.223680	-2.400537
6	-1.871644	2.974772	-2.456201		6	-3.392611	1.568140	-3.189056
1	-1.188170	3.739083	-2.075448		1	-3.429618	1.399406	-4.261355
1	-2.451001	3.406645	-3.274687		6	-2.235946	2.106098	-2.638125
1	-1.255153	2.152055	-2.848706		6	2.203437	2.496606	0.770324
6	-6.451229	1.536525	-0.991788		6	3.157714	1.977037	-0.106985
1	-6.787502	2.160868	-1.822644		6	4.389630	1.609490	0.426148
1	-7.098153	1.732070	-0.132912		1	5.147973	1.218607	-0.245088
1	-6.600402	0.491297	-1.283754		6	4.667714	1.725137	1.783550
6	-2.650873	1.537270	2.309369		6	3.687491	2.250865	2.620501
1	-2.319816	2.472509	2.772984		1	3.889899	2.352953	3.683022
1	-1.789063	0.865877	2.286392		6	2.444700	2.650017	2.137919
1	-3.417437	1.092225	2.944736		6	-3.209271	-2.173876	-1.055458
6	-0.090012	-1.653379	0.106315		1	-2.442995	-1.540956	-1.517626
6	-0.734909	-3.649328	0.984702		1	-2.952311	-3.209653	-1.300824
1	-1.438748	-4.371140	1.363021		1	-4.171616	-1.942002	-1.514950
6	0.595084	-3.713789	0.784144		6	-1.055568	-2.448598	3.494420
1	1.308539	-4.502778	0.952698		1	-0.794013	-3.508757	3.417501
6	-2.511829	-2.004047	0.667135		1	-0.185789	-1.861730	3.187344
6	-3.311039	-1.997465	-0.478361		1	-1.265491	-2.222535	4.540615
6	-4.679180	-1.794721	-0.301275		6	1.398683	-3.183441	-3.068450
1	-5.318509	-1.802720	-1.179449		1	0.604159	-2.443091	-3.211567
6	-5.249092	-1.625024	0.954772		1	1.837329	-3.411917	-4.041471
6	-4.412282	-1.621207	2.068049		1	0.929256	-4.092195	-2.683594

1	-4.837543	-1.479825	3.058623	6	2.877065	-1.796608	1.567709
6	-3.040742	-1.809576	1.946826	1	3.808052	-1.638703	2.115120
6	-2.745302	-2.254916	-1.838487	1	2.231589	-0.929884	1.744886
1	-3.549262	-2.423066	-2.557324	1	2.368347	-2.666256	1.993103
1	-2.098287	-3.137603	-1.833619	6	1.398951	3.183343	3.068580
1	-2.122897	-1.427178	-2.200221	1	0.929049	4.091765	2.683515
6	-6.728994	-1.439730	1.117876	1	0.604730	2.442746	3.212172
1	-6.969101	-0.410099	1.403864	1	1.837807	3.412342	4.041379
1	-7.125411	-2.094649	1.898771	6	2.877033	1.796547	-1.567725
1	-7.261924	-1.656417	0.189997	1	2.231487	0.929873	-1.744879
6	-2.162691	-1.835049	3.164362	1	2.368348	2.666242	-1.993064
1	-1.948488	-2.859844	3.485201	1	3.807987	1.638606	-2.115181
1	-2.648436	-1.322769	3.997027	6	-1.055601	2.448893	-3.494483
1	-1.200231	-1.354306	2.973701	1	-0.185807	1.862024	-3.187445
6	2.329053	-2.203132	-0.091934	1	-1.265564	2.222856	-4.540673
6	2.781898	-2.468038	-1.385090	1	-0.794074	3.509060	-3.417546
6	4.131188	-2.236131	-1.646347	6	-3.208960	2.173760	1.055530
1	4.503669	-2.427633	-2.648746	1	-2.442702	1.540763	1.517620
6	5.009773	-1.792006	-0.665342	1	-2.951991	3.209523	1.300944
6	4.519011	-1.571155	0.619065	1	-4.171295	1.941882	1.515052
1	5.192021	-1.240231	1.403366	6	5.983795	1.263579	2.337439
6	3.178557	-1.765229	0.925483	1	6.317296	1.898785	3.161678
6	1.871449	-2.974627	-2.456244	1	5.903013	0.242007	2.726631
1	1.187853	-3.738805	-2.075439	1	6.761003	1.263518	1.569645
1	2.450727	-3.406645	-3.274709	6	-5.704152	0.599079	-3.018337
1	1.255057	-2.151849	-2.848786	1	-5.988329	1.107125	-3.943726
6	6.451264	-1.536890	-0.992035	1	-5.513087	-0.450072	-3.269598
1	6.787323	-2.161045	-1.823120	1	-6.557474	0.628602	-2.337162
1	7.098230	-1.732852	-0.133282	6	-5.704243	-0.598963	3.018391
1	6.600638	-0.491598	-1.283683	1	-5.986269	-1.104564	3.945762
6	2.651059	-1.537216	2.309298	1	-5.514342	0.451250	3.266121
1	3.417687	-1.092218	2.944617	1	-6.558547	-0.631778	2.338591
1	2.319970	-2.472430	2.772938	6	5.983656	-1.263871	-2.337669
1	1.789293	-0.865773	2.286370	1	6.318216	-1.900621	-3.160300
				1	5.902298	-0.243235	-2.729174
				1	6.760355	-1.261535	-1.569372

TS [Pd(IMes)$_2$(^{2}-O$_2$)] + O$_2$ (OST)

46	0.043657	-0.081639	-0.521739
8	-0.273467	0.253460	2.699294
8	0.542020	-0.079181	3.513807
8	0.232021	-0.815436	-2.374810
8	0.459497	0.380493	-2.880810
6	-0.183032	2.017866	-0.130052
6	0.153199	-1.970764	0.109877
7	-1.283388	2.761132	-0.406331
6	-1.062302	4.110268	-0.199098
1	-1.826617	4.848159	-0.376954
6	0.214887	4.226386	0.225990
1	0.800758	5.088262	0.498163
7	0.730696	2.943982	0.262769
6	-2.532515	2.239375	-0.872023
6	-2.795319	2.242192	-2.244595
6	-4.039864	1.779781	-2.662846
1	-4.258964	1.767516	-3.726909
6	-5.002755	1.339583	-1.759127
6	-4.699774	1.361539	-0.402527

1	-5.440581	1.026242	0.316813
6	-3.461652	1.790107	0.065166
6	2.053716	2.633266	0.703914
6	2.326665	2.680301	2.074684
6	3.612900	2.362045	2.495475
1	3.834068	2.372722	3.559469
6	4.614525	2.026365	1.587297
6	4.308286	2.024365	0.232049
1	5.081335	1.777324	-0.489412
6	3.031857	2.321443	-0.242317
7	1.230493	-2.787050	-0.040968
6	0.951086	-4.078937	0.372013
1	1.692286	-4.859445	0.335577
6	-0.333730	-4.084869	0.781564
1	-0.956131	-4.873874	1.168324
7	-0.805597	-2.791761	0.616460
6	2.503054	-2.386675	-0.560184
6	3.356810	-1.638065	0.248155
6	4.608509	-1.304001	-0.262698
1	5.286566	-0.730027	0.361230
6	5.002720	-1.677739	-1.541045
6	4.116274	-2.420064	-2.318439
1	4.403481	-2.712117	-3.324772
6	2.861603	-2.790898	-1.850262
6	-2.131426	-2.389153	0.962174
6	-3.048752	-2.115902	-0.056284
6	-4.341421	-1.763581	0.320680
1	-5.067059	-1.554911	-0.459203
6	-4.725416	-1.668903	1.653629
6	-3.783984	-1.959157	2.636479
1	-4.066155	-1.898734	3.684338
6	-2.482363	-2.330808	2.314215
6	2.739134	2.312733	-1.708234
1	2.110887	1.461898	-2.003391
1	2.196472	3.214703	-2.007591
1	3.668760	2.265562	-2.278627
6	1.276023	3.080997	3.068448
1	1.217447	4.171074	3.159065
1	0.287340	2.726931	2.772288
1	1.508094	2.677224	4.055526
6	5.989936	1.664150	2.067175
1	5.966023	0.763725	2.690368
1	6.665073	1.474888	1.229624
1	6.422936	2.464934	2.674223
6	2.933425	-1.162658	1.600889
1	2.246630	-0.317542	1.492432
1	2.408518	-1.939259	2.162706
1	3.792231	-0.827027	2.183687
6	1.908810	-3.548711	-2.722933
1	1.025522	-2.930553	-2.908594
1	2.375343	-3.786880	-3.680293
1	1.578099	-4.484347	-2.262636
6	6.338519	-1.264923	-2.086580
1	7.000190	-0.912319	-1.292014
1	6.834686	-2.092978	-2.600175
1	6.226459	-0.452476	-2.812811

6	-2.675226	-2.208770	-1.502399
1	-1.977249	-1.415965	-1.791288
1	-2.172319	-3.155434	-1.722328
1	-3.565673	-2.133074	-2.128967
6	-1.509488	-2.681808	3.401642
1	-1.547054	-3.751880	3.633278
1	-0.482399	-2.446283	3.123449
1	-1.750786	-2.139473	4.318067
6	-6.112926	-1.235392	2.025951
1	-6.503366	-1.817361	2.864699
1	-6.123234	-0.182336	2.331143
1	-6.801997	-1.342713	1.185410
6	-1.759186	2.671773	-3.233245
1	-1.279536	3.610578	-2.942709
1	-0.974520	1.903417	-3.286926
1	-2.201876	2.801450	-4.222580
6	-3.126092	1.712546	1.521847
1	-2.467961	0.857257	1.701897
1	-2.604691	2.606876	1.873190
1	-4.028912	1.576874	2.119923
6	-6.318750	0.801702	-2.239553
1	-6.708756	1.383632	-3.078204
1	-6.207160	-0.232107	-2.588107
1	-7.066225	0.802404	-1.443005

[Pd(IPr)₂] (CSS)

46	0.000042	0.000025	0.000191	**[Pd(IPr)₂] (CSS)** at PBE0/BSI level				
6	0.000698	2.023426	-0.000901	46	0.000025	0.000042	0.000010	
7	1.009199	2.884840	0.338294	6	0.000527	-2.032205	-0.000279	
6	0.640482	4.213568	0.209335	7	1.032890	-2.896610	-0.270028	
1	1.320054	5.018562	0.433790	6	0.651946	-4.224193	-0.170984	
6	-0.637770	4.213609	-0.214643	1	1.339161	-5.031978	-0.360400	
1	-1.316864	5.018646	-0.440374	6	-0.649825	-4.224534	0.170279	
7	-1.007309	2.884887	-0.341439	1	-1.336688	-5.032668	0.359546	
6	2.331973	2.526912	0.739592	7	-1.031405	-2.897129	0.269440	
6	2.668824	2.642709	2.094923	6	2.372562	-2.560517	-0.652004	
6	4.002103	2.441486	2.443183	6	2.714538	-2.647367	-2.009356	
1	4.305826	2.529952	3.479880	6	4.051695	-2.452361	-2.352400	
6	4.946162	2.110597	1.480652	1	4.351854	-2.513357	-3.392811	
1	5.978821	1.949994	1.773476	6	5.003475	-2.177471	-1.382732	
6	4.576445	1.970913	0.152227	1	6.039833	-2.028820	-1.669684	
1	5.321774	1.699590	-0.586922	6	4.636347	-2.087617	-0.048706	
6	3.259950	2.193060	-0.250336	1	5.390179	-1.863700	0.697347	
6	1.598691	2.911443	3.132467	6	3.315399	-2.287191	0.349053	
1	0.850880	3.567206	2.674287	6	1.665429	-2.891052	-3.076654	
6	0.890942	1.602517	3.494292	1	0.822072	-3.403633	-2.604149	
1	0.523683	1.088080	2.599633	6	1.142965	-1.552651	-3.606365	
1	0.042395	1.795886	4.158834	1	0.766431	-0.931143	-2.787114	
1	1.579975	0.926124	4.009583	1	0.331058	-1.712797	-4.323742	
6	2.118527	3.616916	4.379343	1	1.941475	-1.001861	-4.114631	
1	2.663308	4.532551	4.131288	6	2.156298	-3.783390	-4.214701	
1	2.784180	2.972247	4.961951	1	2.567877	-4.725919	-3.841975	
1	1.281508	3.884922	5.030084	1	2.927793	-3.292306	-4.815815	
6	2.859228	2.155825	-1.708399	1	1.326439	-4.017731	-4.887924	
1	1.781921	1.975597	-1.743516	6	2.922654	-2.263325	1.812967	
6	3.512467	1.011998	-2.467550	1	1.883271	-1.922209	1.857919	
1	3.290289	0.059384	-1.987288	6	3.751718	-1.286629	2.639656	
				1	3.745035	-0.286989	2.201215	

1	4.599773	1.120920	-2.534736	1	4.791884	-1.614658	2.741861
1	3.125593	0.976793	-3.490313	1	3.337436	-1.218065	3.649949
6	3.146630	3.504946	-2.370668	6	3.001786	-3.669052	2.418938
1	2.626911	4.321257	-1.861990	1	2.355480	-4.377460	1.895505
1	2.817918	3.494106	-3.414724	1	2.693555	-3.647621	3.469295
1	4.219238	3.725297	-2.354216	1	4.027733	-4.050436	2.376546
6	-2.330194	2.527270	-0.742689	6	-2.371338	-2.561763	0.651186
6	-2.666388	2.641282	-2.098343	6	-2.713692	-2.649544	2.008413
6	-3.999715	2.440783	-2.446830	6	-4.051078	-2.455498	2.351134
1	-4.302931	2.527922	-3.483790	1	-4.351569	-2.517296	3.391413
6	-4.944484	2.112334	-1.484162	6	-5.002686	-2.180543	1.381295
1	-5.977185	1.952303	-1.777151	1	-6.039217	-2.032606	1.668003
6	-4.575420	1.974272	-0.155383	6	-4.635170	-2.089713	0.047450
1	-5.321303	1.704708	0.583843	1	-5.388874	-1.865762	-0.698709
6	-3.258866	2.195709	0.247367	6	-3.314004	-2.288412	-0.350010
6	-1.595556	2.907293	-3.135853	6	-1.664697	-2.893107	3.075839
1	-0.847315	3.563079	-2.678410	1	-0.821340	-3.405892	2.603487
6	-0.888956	1.597085	-3.495244	6	-1.142161	-1.554616	3.605244
1	-0.522749	1.083647	-2.599569	1	-0.765504	-0.933310	2.785852
1	-0.039827	1.788568	-4.159593	1	-0.330322	-1.714650	4.322750
1	-1.578392	0.920616	-4.009902	1	-1.940683	-1.003621	4.113290
6	-2.114153	3.611238	-4.384109	6	-2.155660	-3.785074	4.214108
1	-2.658076	4.527861	-4.137814	1	-2.567382	-4.727657	3.841648
1	-2.780249	2.966293	-4.965906	1	-2.927053	-3.293715	4.815151
1	-1.276594	3.877293	-5.034953	1	-1.325792	-4.019351	4.887348
6	-2.858529	2.159776	1.705574	6	-2.920779	-2.263596	-1.813780
1	-1.781667	1.976924	1.741102	1	-1.881641	-1.921716	-1.858184
6	-3.514711	1.018691	2.466297	6	-3.750277	-1.287174	-2.640359
1	-3.127837	0.983799	3.489066	1	-3.335709	-1.217918	-3.650475
1	-3.295062	0.064893	1.987220	1	-3.744509	-0.287700	-2.201563
1	-4.601718	1.130582	2.533466	1	-4.790164	-1.615931	-2.743053
6	-3.142703	3.510557	2.365840	6	-2.998654	-3.669133	-2.420373
1	-2.814335	3.500331	3.410012	1	-2.690024	-3.647044	-3.470591
1	-4.214743	3.733608	2.348755	1	-4.024327	-4.051304	-2.378554
1	-2.620728	4.324825	1.856217	1	-2.352048	-4.377295	-1.896988
6	-0.000726	-2.023370	0.001242	6	-0.000568	2.032305	0.000430
7	-1.009283	-2.884163	0.341841	7	-1.032898	2.896798	-0.269072
6	-0.640662	-4.213131	0.214978	6	-0.651960	4.224340	-0.169545
1	-1.320289	-5.017714	0.440733	1	-1.339181	5.032192	-0.358642
6	0.637555	-4.213941	-0.209103	6	0.649805	4.224558	0.171730
1	1.316571	-5.019384	-0.433616	1	1.336654	5.032627	0.361294
7	1.007164	-2.885460	-0.338073	7	1.031378	2.897129	0.270395
6	-2.332039	-2.525728	0.742791	6	-2.372585	2.560855	-0.651098
6	-3.260359	-2.193998	-0.247533	6	-3.315301	2.286837	0.349874
6	-4.576930	-1.971996	0.154874	6	-4.636258	2.087304	-0.047897
1	-5.322550	-1.702372	-0.584603	1	-5.390000	1.862809	0.698081
6	-4.946341	-2.109666	1.483591	6	-5.003523	2.177937	-1.381835
1	-5.979056	-1.949246	1.776312	1	-6.039889	2.029304	-1.668782
6	-4.001895	-2.438224	2.446550	6	-4.051865	2.453587	-2.351413
1	-4.305381	-2.525024	3.483457	1	-4.352133	2.515228	-3.391752
6	-2.668567	-2.639289	2.098405	6	-2.714711	2.648527	-2.008355
6	-2.859779	-2.158593	-1.705682	6	-2.922437	2.262253	1.813751
1	-1.782609	-1.977558	-1.741114	1	-1.883069	1.921078	1.858463
6	-3.146191	-3.508838	-2.366068	6	-3.001455	3.667731	2.420320
1	-2.625740	-4.324032	-1.856356	1	-2.355220	4.376337	1.897073
1	-2.817623	-3.499152	-3.410182	1	-2.693055	3.645869	3.470618

Atom	X	Y	Z	Atom	X	Y	Z
1	-4.218620	-3.730026	-2.349180	1	-4.027394	4.049172	2.378247
6	-3.513954	-1.016308	-2.466350	6	-3.751464	1.285239	2.640105
1	-3.292553	-0.062904	-1.987295	1	-3.744684	0.285718	2.201394
1	-4.601168	-1.126218	-2.533418	1	-4.791668	1.613136	2.742362
1	-3.127080	-0.982108	-3.489148	1	-3.337228	1.216433	3.650403
6	-1.598023	-2.905442	3.136172	6	-1.665708	2.892962	-3.075580
1	-0.850008	-3.561713	2.679052	1	-0.822582	3.405790	-2.602940
6	-2.117106	-3.608714	4.384604	6	-2.156926	3.785366	-4.213418
1	-2.661269	-4.525267	4.138576	1	-2.568933	4.727624	-3.840484
1	-2.783114	-2.963315	4.965995	1	-2.928168	3.294099	-4.814712
1	-1.279766	-3.874763	5.035731	1	-1.327133	4.020239	-4.886530
6	-0.890913	-1.595405	3.495191	6	-1.142653	1.554921	-3.605627
1	-0.524479	-1.082391	2.599360	1	-0.765740	0.933425	-2.786545
1	-0.041874	-1.787012	4.159619	1	-0.330898	1.715601	-4.323060
1	-1.580102	-0.918516	4.009622	1	-1.940951	1.003851	-4.113916
6	2.330108	-2.528434	-0.739613	6	2.371279	2.561578	0.652059
6	3.258499	-2.195185	0.250127	6	3.314006	2.288653	-0.349204
6	4.575069	-1.973944	-0.152691	6	4.635116	2.089585	0.048262
1	5.320718	-1.703089	0.586305	1	5.388862	1.865936	-0.697951
6	4.944444	-2.113949	-1.481173	6	5.002518	2.179598	1.382200
1	5.977161	-1.954080	-1.774198	1	6.039004	2.031373	1.668923
6	3.999988	-2.444261	-2.443517	6	4.050842	2.454086	2.352099
1	4.303472	-2.533031	-3.480259	1	4.351225	2.515218	3.392449
6	2.666637	-2.644558	-2.095010	6	2.713516	2.648520	2.009358
6	2.858050	-2.157608	1.708256	6	2.920928	2.264499	-1.813025
1	1.780961	-1.976122	1.743541	1	1.881680	1.923006	-1.857670
6	3.143973	-3.507118	2.370379	6	2.999414	3.670184	-2.419184
1	2.623179	-4.322770	1.861751	1	2.352983	4.378425	-1.895699
1	2.815463	-3.495957	3.414496	1	2.690954	3.648513	-3.469458
1	4.216314	-3.728745	2.353715	1	4.025226	4.051955	-2.377085
6	3.512747	-1.014624	2.467409	6	3.750165	1.288005	-2.639787
1	3.291729	-0.061725	1.987180	1	3.744070	0.288453	-2.201163
1	4.599919	-1.124911	2.534548	1	4.790153	1.616472	-2.742380
1	3.125962	-0.978972	3.490187	1	3.335607	1.219059	-3.649926
6	1.596149	-2.912725	-3.132335	6	1.664498	2.891621	3.076873
1	0.848208	-3.568280	-2.674062	1	0.821040	3.404365	2.604689
6	2.115424	-3.618218	-4.379432	6	2.155380	3.783397	4.215341
1	2.659996	-4.534049	-4.131641	1	2.566912	4.726138	3.843085
1	2.781111	-2.973678	-4.962148	1	2.926913	3.292019	4.816183
1	1.278141	-3.885894	-5.029968	1	1.325532	4.017363	4.888715
6	0.888784	-1.603509	-3.493857	6	1.142222	1.552904	3.605964
1	0.521885	-1.089024	-2.599077	1	0.765722	0.931708	2.786422
1	0.040036	-1.796525	-4.158248	1	0.330324	1.712603	4.323470
1	1.577937	-0.927296	-4.009222	1	1.940841	1.001967	4.113921
[Pd(IPr)$_2$(^{1}-O$_2$)] (OST)				**[Pd(IPr)$_2$(^{1}-O$_2$)] (OSS)**			
46	-0.004541	0.019512	0.023669	46	0.007051	0.040242	0.013273
8	-0.148597	0.070112	-2.200370	8	-0.333372	-0.006319	-1.968412
8	-0.055074	-1.013796	-2.846011	8	0.108833	-1.088323	-2.542858
6	0.377010	-1.988394	0.186480	6	0.445934	-1.965891	0.301181
7	1.521436	-2.675429	-0.099166	7	1.616885	-2.636319	0.126335
6	1.343474	-4.045062	0.003948	6	1.469029	-3.996325	0.338929
1	2.145878	-4.738951	-0.177099	1	2.295315	-4.679805	0.246766
6	0.061512	-4.239658	0.367335	6	0.176439	-4.195814	0.661258
1	-0.500777	-5.137207	0.561309	1	-0.369625	-5.089356	0.911366
7	-0.505019	-2.981782	0.481979	7	-0.428204	-2.950346	0.634244
6	2.801623	-2.105927	-0.388124	6	2.880004	-2.053837	-0.204912

6	3.358075	-2.308392	-1.656294	6	3.430613	-2.321978	-1.462480
6	4.653152	-1.835911	-1.875135	6	4.707935	-1.823065	-1.722695
1	5.111316	-1.980472	-2.847630	1	5.163289	-2.015260	-2.688208
6	5.344733	-1.165575	-0.882922	6	5.383518	-1.066580	-0.782211
1	6.344041	-0.789628	-1.077846	1	6.368576	-0.672238	-1.010611
6	4.763686	-0.968245	0.362701	6	4.805111	-0.804024	0.452783
1	5.314763	-0.436936	1.128694	1	5.342934	-0.203751	1.176250
6	3.491658	-1.453775	0.648183	6	3.550563	-1.309154	0.778505
6	2.623964	-3.031015	-2.767513	6	2.708479	-3.140909	-2.512434
1	1.584506	-3.159045	-2.456974	1	1.678126	-3.282005	-2.177996
6	2.598690	-2.224905	-4.064978	6	2.630334	-2.418856	-3.855846
1	2.095268	-1.270007	-3.917083	1	2.059668	-1.496098	-3.743389
1	2.044333	-2.777276	-4.829416	1	2.110043	-3.052179	-4.580948
1	3.606582	-2.044603	-4.452155	1	3.623338	-2.198989	-4.261568
6	3.240805	-4.410808	-3.011119	6	3.370530	-4.512311	-2.668501
1	3.260735	-5.021403	-2.104298	1	3.420828	-5.057675	-1.721613
1	4.272925	-4.318208	-3.364676	1	4.394933	-4.410666	-3.041707
1	2.672721	-4.953435	-3.772551	1	2.812688	-5.124730	-3.383089
6	2.895683	-1.340792	2.037424	6	2.953116	-1.121580	2.159180
1	1.845047	-1.056981	1.909381	1	1.887827	-0.908984	2.019823
6	3.548959	-0.267695	2.894217	6	3.547660	0.050125	2.925015
1	3.543278	0.702243	2.396138	1	3.490685	0.975113	2.350236
1	4.582880	-0.523137	3.151079	1	4.594011	-0.128696	3.194892
1	2.999362	-0.169692	3.834584	1	2.995667	0.193261	3.858281
6	2.952304	-2.687267	2.765726	6	3.082474	-2.403205	2.987968
1	2.426476	-3.476623	2.225730	1	2.597679	-3.256681	2.510756
1	2.495370	-2.598484	3.756559	1	2.623060	-2.264538	3.971957
1	3.991968	-3.003699	2.901232	1	4.137697	-2.652967	3.140058
6	-1.864832	-2.821381	0.892735	6	-1.804708	-2.773464	0.980505
6	-2.146349	-2.829437	2.266144	6	-2.131109	-2.692587	2.339544
6	-3.485683	-2.818637	2.644522	6	-3.482681	-2.638208	2.672012
1	-3.745646	-2.831808	3.697080	1	-3.778589	-2.584789	3.713872
6	-4.495384	-2.780907	1.690936	6	-4.455278	-2.636995	1.682282
1	-5.533656	-2.770888	2.007291	1	-5.503810	-2.587039	1.958945
6	-4.183992	-2.746527	0.342168	6	-4.097812	-2.687093	0.343959
1	-4.978959	-2.706573	-0.394844	1	-4.868286	-2.663987	-0.417400
6	-2.857251	-2.779200	-0.087523	6	-2.760260	-2.771338	-0.040977
6	-1.032119	-2.793235	3.290771	6	-1.050923	-2.596458	3.397421
1	-0.146190	-3.244270	2.833661	1	-0.150749	-3.075748	3.000975
6	-0.684464	-1.339708	3.621227	6	-0.709161	-1.126291	3.652447
1	-0.449128	-0.778803	2.710309	1	-0.451015	-0.618844	2.716939
1	0.179565	-1.290101	4.291689	1	0.137882	-1.036924	4.340015
1	-1.528070	-0.846066	4.113397	1	-1.563851	-0.602310	4.090467
6	-1.345875	-3.585814	4.555178	6	-1.409756	-3.309473	4.696919
1	-1.641267	-4.612830	4.323316	1	-1.693203	-4.350264	4.518149
1	-2.150490	-3.123894	5.135330	1	-2.237721	-2.817026	5.215738
1	-0.463464	-3.621632	5.200365	1	-0.552476	-3.300647	5.375983
6	-2.520143	-2.807165	-1.559362	6	-2.354255	-2.903887	-1.491236
1	-1.442616	-2.667156	-1.667594	1	-1.384809	-2.412501	-1.632598
6	-3.178284	-1.651224	-2.300261	6	-3.318813	-2.213553	-2.444066
1	-2.849204	-1.641666	-3.342312	1	-2.889707	-2.212550	-3.449008
1	-2.890760	-0.700965	-1.848943	1	-3.483422	-1.176933	-2.150153
1	-4.270635	-1.721287	-2.287651	1	-4.288550	-2.721901	-2.498874
6	-2.890022	-4.158346	-2.171830	6	-2.202394	-4.378927	-1.874843
1	-2.606321	-4.184555	-3.228015	1	-1.884271	-4.458725	-2.918588
1	-3.967923	-4.340605	-2.106107	1	-3.153858	-4.911315	-1.765685

1	-2.380322	-4.981841	-1.662813	1	-1.455670	-4.889213	-1.262281
6	-0.385697	2.033139	-0.020654	6	-0.448085	2.019500	-0.138861
7	-1.531046	2.664011	-0.405278	7	-1.618458	2.572173	-0.552686
6	-1.366173	4.036523	-0.490272	6	-1.498246	3.936159	-0.758081
1	-2.173513	4.690638	-0.771340	1	-2.330327	4.537324	-1.081761
6	-0.087697	4.290549	-0.150074	6	-0.223860	4.259050	-0.461244
1	0.466049	5.211614	-0.080911	1	0.301107	5.199073	-0.480539
7	0.488615	3.065300	0.138312	7	0.396260	3.081905	-0.079360
6	-2.788629	2.041483	-0.683278	6	-2.859225	1.886180	-0.752563
6	-3.557345	1.570049	0.392976	6	-3.615528	1.528342	0.373611
6	-4.813796	1.049764	0.097887	6	-4.862269	0.953555	0.145879
1	-5.428125	0.652557	0.896441	1	-5.468856	0.640967	0.986783
6	-5.297944	1.039917	-1.203511	6	-5.343527	0.777414	-1.144215
1	-6.287492	0.643296	-1.406925	1	-6.324095	0.338616	-1.298217
6	-4.520729	1.520207	-2.241863	6	-4.572738	1.141907	-2.234436
1	-4.901522	1.491948	-3.257214	1	-4.950107	0.980018	-3.238431
6	-3.237881	2.016088	-2.007741	6	-3.300880	1.688789	-2.063839
6	-3.048967	1.665854	1.818607	6	-3.101675	1.788736	1.776622
1	-2.001321	1.344190	1.801679	1	-2.042898	1.506403	1.781215
6	-3.102586	3.107615	2.334039	6	-3.206178	3.271942	2.145274
1	-2.505727	3.791694	1.728874	1	-2.642170	3.912590	1.465755
1	-2.721770	3.152013	3.359225	1	-2.818756	3.435851	3.155839
1	-4.135195	3.472154	2.342027	1	-4.252140	3.595382	2.128820
6	-3.788521	0.753472	2.785493	6	-3.797858	0.950818	2.839321
1	-3.789215	-0.281379	2.441934	1	-3.763169	-0.112171	2.597593
1	-4.825597	1.073937	2.933818	1	-4.844704	1.246471	2.967386
1	-3.299420	0.785721	3.763090	1	-3.302702	1.098925	3.803294
6	-2.397541	2.518268	-3.164408	6	-2.462706	2.063512	-3.268313
1	-1.388625	2.707352	-2.789322	1	-1.451803	2.282993	-2.915553
6	-2.964411	3.830480	-3.711506	6	-3.025981	3.313062	-3.949458
1	-3.035937	4.600559	-2.938535	1	-3.089533	4.162408	-3.263742
1	-3.968973	3.679489	-4.119449	1	-4.033194	3.124456	-4.334945
1	-2.329684	4.215021	-4.515359	1	-2.393069	3.605802	-4.792513
6	-2.268620	1.481724	-4.279553	6	-2.337272	0.914990	-4.267726
1	-1.801828	0.567370	-3.914094	1	-1.882257	0.041845	-3.800553
1	-1.641020	1.882515	-5.081466	1	-1.698239	1.224671	-5.100326
1	-3.241150	1.234053	-4.716597	1	-3.308493	0.633128	-4.687232
6	1.866725	2.950715	0.499199	6	1.781464	3.030863	0.271259
6	2.790787	2.629209	-0.498353	6	2.700947	2.647625	-0.708668
6	4.138162	2.613231	-0.139472	6	4.051271	2.686174	-0.361867
1	4.882777	2.352445	-0.882703	1	4.794329	2.379566	-1.088706
6	4.535105	2.934653	1.148464	6	4.452693	3.116966	0.892369
1	5.589751	2.930347	1.404984	1	5.509471	3.153063	1.137344
6	3.593062	3.253842	2.117728	6	3.513744	3.493873	1.843877
1	3.920531	3.491543	3.123216	1	3.845401	3.816417	2.824044
6	2.233666	3.255840	1.816335	6	2.152226	3.445388	1.556919
6	2.350064	2.380278	-1.923521	6	2.249869	2.273667	-2.103152
1	1.304178	2.066167	-1.902365	1	1.221088	1.909314	-2.042039
6	2.448373	3.672922	-2.737170	6	2.278722	3.506192	-3.010462
1	1.846685	4.473145	-2.297396	1	1.648492	4.311056	-2.621856
1	2.092088	3.505215	-3.758073	1	1.915394	3.246833	-4.009376
1	3.485271	4.021392	-2.790935	1	3.298346	3.894010	-3.108862
6	3.116806	1.247366	-2.587727	6	3.057431	1.130286	-2.697054
1	3.046643	0.336581	-1.993280	1	3.030421	0.261168	-2.040428
1	4.175695	1.485514	-2.732604	1	4.103193	1.402094	-2.876706
1	2.687230	1.041847	-3.571409	1	2.621055	0.834821	-3.653841

6	1.177682	3.512675	2.871485		6	1.098938	3.761141	2.599160
1	0.336749	4.017023	2.384153		1	0.247128	4.217057	2.083686
6	1.653479	4.412663	4.005702		6	1.567736	4.746271	3.663201
1	2.072407	5.350612	3.630441		1	1.970512	5.660477	3.218532
1	2.414720	3.921140	4.619386		1	2.339950	4.311051	4.305041
1	0.815205	4.653469	4.665231		1	0.729943	5.021923	4.309529
6	0.653875	2.179646	3.413267		6	0.599050	2.463418	3.240783
1	0.318500	1.527902	2.601357		1	0.262709	1.751498	2.481819
1	-0.185472	2.343242	4.096531		1	-0.236183	2.663374	3.919197
1	1.442781	1.654360	3.959549		1	1.400201	1.987745	3.813599

[Pd(IPr)₂(²-O₂)] (CSS)					[Pd(IPr)₂(²-O₂)] (CSS) at PBE0/BSI level			
46	0.056274	-0.228913	-0.856800		46	0.000781	-0.000812	-0.858959
8	0.255369	-1.274520	-2.553443		8	0.203916	-0.656058	-2.743579
8	-0.018185	0.041187	-2.839945		8	-0.200685	0.652311	-2.744468
7	-0.533874	-2.623058	0.971347		7	-0.234821	-2.844979	0.356900
7	1.556734	-2.434562	0.583837		7	1.798309	-2.361246	-0.091098
7	0.501266	2.764915	-0.392921		7	0.234346	2.846073	0.350528
7	-1.567339	2.316393	-0.664363		7	-1.798368	2.360391	-0.097390
6	0.382872	-1.743470	0.477142		6	0.566027	-1.775731	0.062083
6	0.048436	-3.821358	1.352794		6	0.467506	-4.037571	0.366653
1	-0.534133	-4.628800	1.762967		1	-0.012613	-4.977890	0.578711
6	1.364490	-3.703047	1.102870		6	1.745171	-3.731783	0.083126
1	2.183270	-4.386093	1.248196		1	2.620219	-4.351577	-0.010991
6	-1.934466	-2.409091	1.176835		6	-1.624932	-2.858820	0.711377
6	-2.349722	-2.150709	2.491421		6	-1.941799	-3.004965	2.069697
6	-3.720388	-2.101946	2.733199		6	-3.282139	-3.191790	2.405709
1	-4.083120	-1.932128	3.740143		1	-3.558047	-3.316312	3.448309
6	-4.627843	-2.270553	1.698010		6	-4.263400	-3.216466	1.427645
6	-4.185325	-2.505239	0.406893		6	-3.921615	-3.060883	0.092822
1	-4.907584	-2.626064	-0.390679		1	-4.698789	-3.081214	-0.662318
6	-2.825348	-2.604567	0.114835		6	-2.594183	-2.898166	-0.302010
6	-1.330982	-1.929389	3.593964		6	-0.887411	-2.985168	3.161159
1	-0.516611	-2.643829	3.434002		1	0.088738	-2.858181	2.686648
6	-2.342913	-2.963671	-1.275227		6	-2.218924	-2.854750	-1.769373
1	-1.447916	-2.370749	-1.493711		1	-1.301617	-2.268207	-1.876554
6	2.864543	-1.987997	0.202948		6	3.057158	-1.729941	-0.381638
6	3.389317	-2.428050	-1.017363		6	3.544589	-1.760596	-1.696879
6	4.705741	-2.072220	-1.313258		6	4.819911	-1.238289	-1.919213
1	5.142586	-2.394271	-2.251794		1	5.224911	-1.245586	-2.925216
6	5.451099	-1.302240	-0.438210		6	5.572542	-0.712532	-0.883783
6	4.903280	-0.879466	0.764484		6	5.076281	-0.718191	0.411045
1	5.498462	-0.273067	1.435605		1	5.681934	-0.315660	1.214300
6	3.604116	-1.228534	1.122859		6	3.818898	-1.245252	0.695672
6	2.605343	-3.302014	-1.973744		6	2.786530	-2.398707	-2.844944
1	1.548384	-3.225367	-1.709062		1	1.740323	-2.495662	-2.547813
6	3.028785	-0.843760	2.473352		6	3.339045	-1.365815	2.131139
1	1.995144	-0.524592	2.301150		1	2.249152	-1.257017	2.121479
6	-0.375375	1.719229	-0.356941		6	-0.565998	1.775685	0.058436
6	-0.116554	3.952182	-0.745799		6	-0.468227	4.038547	0.355604
1	0.432144	4.875187	-0.823804		1	0.011554	4.979662	0.564875
6	-1.419477	3.667226	-0.922612		6	-1.745625	3.731523	0.072140
1	-2.255065	4.287237	-1.197703		1	-2.620770	4.350742	-0.024754
6	1.872927	2.776313	0.015009		6	1.624144	2.861437	0.706196
6	2.871503	2.448641	-0.908236		6	2.594113	2.899228	-0.306473
6	4.194145	2.611629	-0.498528		6	3.921172	3.063770	0.088921
1	4.994627	2.351568	-1.181351		1	4.698833	3.083155	-0.665768

6	4.499755	3.123441	0.753411	6	4.261853	3.222549	1.423628
6	3.486835	3.455593	1.640692	6	3.279843	3.199262	2.401024
1	3.735228	3.850207	2.621020	1	3.554897	3.326247	3.443552
6	2.149694	3.273385	1.294548	6	1.939908	3.010718	2.064449
6	2.531792	2.030227	-2.319536	6	2.220046	2.852985	-1.774008
1	1.541501	1.568155	-2.320209	1	1.300026	2.270645	-1.880321
6	1.050327	3.623297	2.276645	6	0.884714	2.992634	3.155146
1	0.091215	3.403571	1.802075	1	-0.090904	2.863264	2.680170
6	-2.855102	1.689795	-0.718366	6	-3.057007	1.727751	-0.385987
6	-3.390254	1.362097	-1.968788	6	-3.544529	1.754379	-1.701276
6	-4.680460	0.829825	-1.994107	6	-4.819783	1.231161	-1.921970
1	-5.125535	0.568496	-2.948019	1	-5.224873	1.235450	-2.927963
6	-5.395633	0.635710	-0.826680	6	-5.572271	0.708404	-0.884926
6	-4.848192	0.993130	0.397164	6	-5.075951	0.718078	0.409863
1	-5.425181	0.839343	1.300122	1	-5.681549	0.317921	1.214340
6	-3.574756	1.547028	0.480570	6	-3.818648	1.246204	0.692851
6	-2.664368	1.645991	-3.267398	6	-2.786801	2.389243	-2.851351
1	-1.613651	1.830219	-3.036373	1	-1.740698	2.487983	-2.554452
6	-3.018356	2.032823	1.807577	6	-3.338830	1.371372	2.127960
1	-1.963121	1.740479	1.844440	1	-2.248994	1.261827	2.118814
6	1.062400	5.112066	2.620593	6	0.848910	4.314769	3.924445
1	0.961144	5.727560	1.722698	1	0.675471	5.162696	3.256173
1	0.235343	5.355359	3.294408	1	0.046905	4.300846	4.668896
1	1.994650	5.398210	3.117274	1	1.789961	4.495476	4.453273
6	1.131630	2.761582	3.534649	6	1.081036	1.810994	4.106032
1	2.055626	2.948325	4.090585	1	2.030331	1.884805	4.645909
1	0.290400	2.980917	4.199454	1	0.276984	1.784295	4.848367
1	1.097590	1.700681	3.279786	1	1.075203	0.864176	3.560530
6	2.478896	3.259889	-3.230211	6	1.953656	4.269104	-2.297791
1	1.747302	3.993290	-2.880260	1	1.148742	4.765150	-1.749043
1	3.455828	3.753282	-3.279606	1	2.852560	4.890311	-2.216786
1	2.194083	2.961210	-4.243218	1	1.662025	4.228643	-3.351604
6	3.485664	0.983702	-2.877924	6	3.266803	2.158936	-2.638694
1	3.097800	0.615878	-3.830858	1	2.865981	2.019996	-3.645989
1	4.488648	1.386097	-3.059582	1	4.187401	2.746575	-2.729603
1	3.572083	0.132724	-2.201559	1	3.520827	1.174685	-2.240536
6	-3.101172	3.559603	1.928164	6	-3.681554	2.753596	2.699665
1	-2.519149	4.076775	1.166035	1	-3.217667	3.565414	2.137633
1	-4.142279	3.888356	1.847265	1	-4.765371	2.909267	2.691427
1	-2.723208	3.877530	2.905282	1	-3.339121	2.828796	3.737008
6	-3.721143	1.421444	3.013478	6	-3.906734	0.299360	3.051553
1	-3.197561	1.707964	3.930058	1	-3.420157	0.360014	4.029096
1	-4.747760	1.791257	3.104706	1	-4.979349	0.440714	3.220707
1	-3.749900	0.333378	2.956979	1	-3.748794	-0.702852	2.651840
6	-3.254555	2.896652	-3.925818	6	-3.352036	3.783055	-3.149814
1	-2.703452	3.139193	-4.839221	1	-2.782183	4.256762	-3.955072
1	-4.303534	2.737039	-4.196488	1	-4.397509	3.719887	-3.470292
1	-3.213358	3.767451	-3.265815	1	-3.312177	4.442708	-2.278739
6	-2.691605	0.465731	-4.232836	6	-2.800246	1.531605	-4.115258
1	-2.192497	-0.394635	-3.789771	1	-2.363931	0.553328	-3.915153
1	-3.711586	0.196314	-4.527130	1	-3.809913	1.413684	-4.523249
1	-2.143599	0.728345	-5.141970	1	-2.189664	2.011574	-4.885461
6	-1.958170	-4.444078	-1.361150	6	-1.945010	-4.271051	-2.288793
1	-1.148280	-4.703780	-0.677118	1	-1.137782	-4.761341	-1.738357
1	-2.818546	-5.083026	-1.133757	1	-2.840803	-4.896561	-2.206376
1	-1.619543	-4.676508	-2.374975	1	-1.653147	-4.232132	-3.342593

6	-3.359288	-2.638162	-2.361612	6	-3.268357	-2.168974	-2.637437
1	-2.889456	-2.758183	-3.340567	1	-2.866821	-2.030495	-3.644510
1	-4.225917	-3.308337	-2.326725	1	-4.185281	-2.762364	-2.728210
1	-3.711821	-1.608551	-2.282669	1	-3.528888	-1.185123	-2.242427
6	-1.879646	-2.182945	4.992985	6	-0.853714	-4.305248	3.934049
1	-2.340004	-3.171357	5.076830	1	-0.680939	-5.155198	3.268170
1	-1.068899	-2.122973	5.724208	1	-0.052137	-4.290315	4.678938
1	-2.625449	-1.433562	5.276591	1	-1.795296	-4.483380	4.462795
6	-0.718707	-0.527878	3.507287	6	-1.083075	-1.800663	4.108605
1	0.129938	-0.445843	4.193779	1	-0.279583	-1.772830	4.851508
1	-0.372014	-0.296591	2.496895	1	-1.075645	-0.855407	3.560402
1	-1.453280	0.228714	3.792845	1	-2.032896	-1.871806	4.647913
6	3.011988	-2.032551	3.440944	6	3.682631	-2.745867	2.707536
1	2.394415	-2.857349	3.086593	1	3.219465	-3.559865	2.148071
1	4.029079	-2.406734	3.596580	1	4.766559	-2.900792	2.700023
1	2.617961	-1.717084	4.412377	1	3.340030	-2.817880	3.745040
6	3.772799	0.307335	3.135344	6	3.906211	-0.290257	3.051039
1	3.851547	1.170398	2.475325	1	3.747663	0.710459	2.647853
1	3.241177	0.616248	4.038869	1	3.419657	-0.347812	4.028781
1	4.780640	0.007295	3.441459	1	4.978918	-0.430311	3.220723
6	2.727243	-2.838608	-3.422820	6	2.800886	-1.545465	-4.111823
1	3.753378	-2.922462	-3.795660	1	3.810687	-1.429927	-4.520137
1	2.093996	-3.464146	-4.058218	1	2.189975	-2.027583	-4.880414
1	2.376248	-1.811875	-3.519682	1	2.365463	-0.566108	-3.915152
6	3.045668	-4.762372	-1.838825	6	3.350705	-3.793990	-3.138601
1	2.453275	-5.399008	-2.502709	1	2.780438	-4.270076	-3.942158
1	4.099583	-4.875820	-2.113739	1	4.396185	-3.732648	-3.459425
1	2.926553	-5.137335	-0.819077	1	3.310471	-4.450553	-2.265218
1	-5.692756	-2.220114	1.901799	1	-5.302748	-3.359199	1.706634
1	6.468590	-1.024572	-0.694008	1	6.558223	-0.303904	-1.083484
1	-6.393148	0.209765	-0.866570	1	-6.557915	0.299058	-1.083328
1	5.536990	3.261734	1.041785	1	5.300876	3.366716	1.703104
[Pd(IPr)₂(¹-O₂)₂] (OST)				**[Pd(IPr)₂(¹-O₂)₂] (OST)** at PBE0/BSI level			
46	-0.025727	0.000172	0.000014	46	-0.007721	0.000083	-0.000061
8	0.011872	0.092265	-2.018443	8	0.031064	0.036747	-2.021709
8	-0.638204	-0.823487	-2.659014	8	-0.649592	-0.875930	-2.634955
8	0.006889	-0.093084	2.018418	8	0.028259	-0.037406	2.021553
8	-0.636619	0.827201	2.659091	8	-0.649578	0.877453	2.634655
6	-0.012626	2.045176	0.078082	6	-0.002662	2.065137	-0.017550
7	0.970349	2.834965	0.574062	7	0.981358	2.897224	0.413114
6	0.567710	4.157755	0.641054	6	0.581344	4.220520	0.358528
1	1.220369	4.931286	1.007237	1	1.232820	5.023522	0.658054
6	-0.689975	4.200661	0.157884	6	-0.674711	4.223809	-0.126415
1	-1.381005	5.015886	0.028652	1	-1.361071	5.028857	-0.326282
7	-1.021023	2.903942	-0.194763	7	-1.012714	2.903831	-0.362518
6	2.315937	2.435566	0.863287	6	2.330113	2.556442	0.776497
6	2.756213	2.466972	2.189435	6	2.716821	2.683382	2.117160
6	4.108332	2.212142	2.422901	6	4.068902	2.506286	2.415032
1	4.483182	2.237902	3.440576	1	4.401537	2.604813	3.443034
6	4.965889	1.903695	1.381586	6	4.985883	2.197260	1.425640
1	6.011327	1.694811	1.584868	1	6.032138	2.059581	1.679995
6	4.491852	1.847472	0.078006	6	4.570141	2.055458	0.109543
1	5.168982	1.588394	-0.726491	1	5.295769	1.804244	-0.655032
6	3.161675	2.131387	-0.216555	6	3.238029	2.245464	-0.250981
6	1.833555	2.772102	3.349953	6	1.744011	3.022558	3.229817
1	0.808946	2.793958	2.971996	1	0.731157	2.965004	2.824260

6	1.883055	1.671716	4.408995	6	1.815018	2.008851	4.372923
1	1.608510	0.710223	3.974768	1	1.618350	1.000055	4.007849
1	1.169111	1.893380	5.207065	1	1.055196	2.244524	5.123502
1	2.877102	1.588619	4.860543	1	2.790698	2.024853	4.869973
6	2.158889	4.135820	3.961755	6	1.981528	4.442573	3.752003
1	2.096789	4.940091	3.223020	1	1.897697	5.191731	2.959487
1	3.171693	4.149001	4.377258	1	2.979735	4.538559	4.191716
1	1.460630	4.366224	4.771678	1	1.249451	4.689629	4.526740
6	2.667176	2.177106	-1.648890	6	2.813579	2.191668	-1.706985
1	1.659239	1.755112	-1.668173	1	1.783335	1.826650	-1.744235
6	3.500041	1.336484	-2.604619	6	3.643039	1.224048	-2.543622
1	3.604173	0.311918	-2.246608	1	3.672605	0.229350	-2.095572
1	4.499980	1.756987	-2.758099	1	4.671856	1.574496	-2.680936
1	3.007986	1.302487	-3.579814	1	3.198555	1.130448	-3.538156
6	2.593029	3.623224	-2.149002	6	2.851991	3.593546	-2.327185
1	1.923568	4.238279	-1.544254	1	2.204049	4.296561	-1.798147
1	2.224169	3.644343	-3.178968	1	2.521568	3.554306	-3.369940
1	3.586021	4.084486	-2.134761	1	3.871349	3.993801	-2.310514
6	-2.278494	2.592181	-0.810239	6	-2.291987	2.571545	-0.932429
6	-2.360682	2.624854	-2.209417	6	-2.417246	2.555264	-2.330935
6	-3.621557	2.454058	-2.775382	6	-3.695344	2.368953	-2.854415
1	-3.725340	2.470687	-3.854238	1	-3.829016	2.347778	-3.930221
6	-4.743176	2.261912	-1.981710	6	-4.796293	2.215432	-2.025607
1	-5.715581	2.133026	-2.446039	1	-5.782082	2.074590	-2.457604
6	-4.624630	2.216056	-0.602898	6	-4.640745	2.237621	-0.649741
1	-5.503591	2.048006	0.010704	1	-5.507160	2.118171	-0.007810
6	-3.385778	2.382140	0.015075	6	-3.385478	2.421506	-0.069838
6	-1.150645	2.898731	-3.077133	6	-1.243045	2.804005	-3.258508
1	-0.264285	2.629866	-2.498871	1	-0.327537	2.600657	-2.697441
6	-1.120799	2.050651	-4.345062	6	-1.232024	1.876437	-4.472572
1	-1.184459	0.986692	-4.109359	1	-1.243173	0.827516	-4.169909
1	-0.178246	2.222398	-4.873973	1	-0.321106	2.050436	-5.053959
1	-1.929255	2.317478	-5.033531	1	-2.079004	2.068359	-5.139513
6	-1.072093	4.389969	-3.415194	6	-1.223715	4.270846	-3.703928
1	-1.012001	5.007081	-2.514910	1	-1.166290	4.956801	-2.854529
1	-1.954859	4.704600	-3.981257	1	-2.128392	4.514894	-4.270647
1	-0.186830	4.597323	-4.023979	1	-0.360223	4.461812	-4.348895
6	-3.268233	2.343701	1.521082	6	-3.248707	2.510183	1.435787
1	-2.212361	2.425001	1.786357	1	-2.186613	2.468204	1.687098
6	-3.740855	1.000389	2.066091	6	-3.898333	1.322539	2.140786
1	-3.586959	0.955831	3.147479	1	-3.710725	1.382612	3.216503
1	-3.173662	0.182824	1.619057	1	-3.480433	0.380131	1.783889
1	-4.803276	0.830608	1.863979	1	-4.983143	1.297780	1.991191
6	-4.018959	3.510522	2.161692	6	-3.820081	3.834955	1.949713
1	-3.891629	3.490839	3.248046	1	-3.685302	3.910902	3.033027
1	-5.091826	3.460391	1.948790	1	-4.891877	3.911691	1.737654
1	-3.652120	4.473639	1.794286	1	-3.328114	4.696434	1.488312
6	-0.017476	-2.044917	-0.078106	6	-0.003440	-2.064997	0.017483
7	-1.027676	-2.901580	0.194681	7	-1.013660	-2.903397	0.362668
6	-0.699308	-4.198985	-0.157959	6	-0.675967	-4.223500	0.126771
1	-1.392040	-5.012772	-0.028767	1	-1.362468	-5.028382	0.326844
6	0.558506	-4.158697	-0.641030	6	0.580048	-4.220575	-0.358287
1	1.209592	-4.933569	-1.007167	1	1.231323	-5.023762	-0.657760
7	0.963881	-2.836753	-0.573983	7	0.980340	-2.897379	-0.413140
6	-2.284649	-2.587228	0.809832	6	-2.292964	-2.570758	0.932305
6	-3.391294	-2.375116	-0.015809	6	-3.386237	-2.420828	0.069418

6	-4.629979	-2.206502	0.601815	6	-4.641635	-2.236770	0.648982
1	-5.508473	-2.036885	-0.012025	1	-5.507892	-2.117434	0.006814
6	-4.748980	-2.251916	1.980607	6	-4.797501	-2.214299	2.024808
1	-5.721253	-2.121042	2.444660	1	-5.783383	-2.073331	2.456551
6	-3.627975	-2.446301	2.774590	6	-3.696755	-2.367703	2.853906
1	-3.732070	-2.462692	3.853417	1	-3.830686	-2.346304	3.929674
6	-2.367297	-2.619719	2.208991	6	-2.418541	-2.554222	2.330781
6	-3.273327	-2.337425	-1.521819	6	-3.249119	-2.509881	-1.436160
1	-2.217510	-2.420321	-1.786802	1	-2.186968	-2.467941	-1.687271
6	-4.025557	-3.503478	-2.162077	6	-3.820345	-3.834835	-1.949778
1	-3.660057	-4.466952	-1.794286	1	-3.328463	-4.696124	-1.487925
1	-3.898102	-3.484371	-3.248427	1	-3.685303	-3.911177	-3.033032
1	-5.098373	-3.451820	-1.949280	1	-4.892186	-3.911508	-1.737934
6	-3.743867	-0.993711	-2.067597	6	-3.898589	-1.322456	-2.141658
1	-3.175428	-0.176819	-1.620963	1	-3.480533	-0.379960	-1.785177
1	-4.806050	-0.822158	-1.865704	1	-4.983393	-1.297484	-1.992077
1	-3.589806	-0.949978	-3.148998	1	-3.710991	-1.383013	-3.217353
6	-1.158153	-2.896204	3.077115	6	-1.244590	-2.802878	3.258691
1	-0.271000	-2.629370	2.499144	1	-0.328935	-2.599742	2.697804
6	-1.083074	-4.387580	3.415341	6	-1.225520	-4.269602	3.704504
1	-1.024094	-5.004903	2.515118	1	-1.167968	-4.955791	2.855299
1	-1.966716	-4.700204	3.981147	1	-2.130344	-4.513420	4.271086
1	-0.198474	-4.596884	4.024424	1	-0.362195	-4.460488	4.349719
6	-1.126886	-2.048022	4.344947	6	-1.233807	-1.874947	4.472478
1	-1.188113	-0.983963	4.109076	1	-1.244801	-0.826131	4.169460
1	-0.184899	-2.221745	4.874233	1	-0.323050	-2.048807	5.054163
1	-1.936166	-2.312984	5.033165	1	-2.080973	-2.066617	5.139255
6	2.310380	-2.440228	-0.862894	6	2.329266	-2.557063	-0.776316
6	3.156531	-2.137973	0.217169	6	3.237263	-2.247154	0.251401
6	4.487494	-1.857394	-0.077053	6	4.569571	-2.057988	-0.108856
1	5.165023	-1.599897	0.727613	1	5.295301	-1.807654	0.655917
6	4.961761	-1.914931	-1.380488	6	4.985370	-2.199570	-1.424953
1	6.007781	-1.708707	-1.583486	1	6.031762	-2.062585	-1.679119
6	4.103726	-2.221273	-2.422029	6	4.068289	-2.507516	-2.414601
1	4.478794	-2.247957	-3.439599	1	4.401008	-2.605884	-3.442592
6	2.750916	-2.472748	-2.188925	6	2.716047	-2.683814	-2.116973
6	2.661544	-2.182319	1.649406	6	2.812681	-2.193613	1.707368
1	1.654862	-1.757275	1.668525	1	1.782283	-1.829039	1.744538
6	2.583030	-3.628229	2.149465	6	2.851598	-3.595498	2.327508
1	1.911944	-4.241349	1.544553	1	2.204000	-4.298741	1.798341
1	2.213873	-3.648286	3.179346	1	2.521027	-3.556450	3.370224
1	3.574688	-4.092351	2.135451	1	3.871110	-3.995368	2.310946
6	3.496774	-1.344284	2.605349	6	3.641656	-1.225613	2.544051
1	3.604022	-0.319992	2.247481	1	3.670831	-0.230952	2.095908
1	4.495430	-1.767799	2.758899	1	4.670610	-1.575604	2.681466
1	3.004713	-1.308944	3.580495	1	3.197048	-1.132133	3.538544
6	1.827813	-2.775655	-3.349696	6	1.743142	-3.022043	-3.229848
1	0.803050	-2.794848	-2.972017	1	0.730277	-2.963996	-2.824378
6	2.149816	-4.140259	-3.961279	6	1.979823	-4.442060	-3.752410
1	2.085557	-4.944308	-3.222492	1	1.895394	-5.191395	-2.960122
1	3.162656	-4.156019	-4.376604	1	2.978027	-4.538554	-4.192020
1	1.451125	-4.368967	-4.771307	1	1.247695	-4.688410	-4.527323
6	1.880483	-1.675502	-4.408819	6	1.814943	-2.008027	-4.372617
1	1.608216	-0.713295	-3.974746	1	1.618801	-0.999244	-4.007228
1	1.166302	-1.895452	-5.207155	1	1.055118	-2.243004	-5.123413
1	2.874920	-1.594961	-4.859977	1	2.790709	-2.024465	-4.869477

TS$_{I B}$ (NHC = IPr, OST)				TS [Pd(IPr)$_2$(^{2}-O$_2$)] + O$_2$ (OST)			
46	0.040970	-0.122008	-0.360244	46	0.081796	-0.078945	-0.455624
8	0.376320	-0.617672	-2.234107	8	-0.083710	0.129640	2.567995
8	0.042743	0.550441	-2.734985	8	0.649682	-0.516603	3.270018
6	-0.420576	1.998270	-0.155536	8	0.425810	-0.620194	-2.348360
6	0.390410	-2.037282	0.110290	8	0.058732	0.596264	-2.687219
7	-1.564082	2.621447	-0.553188	6	-0.379317	2.028520	-0.088395
6	-1.389547	3.986408	-0.692331	6	0.385514	-1.955354	0.204797
1	-2.189332	4.636074	-1.003781	7	-1.510492	2.655106	-0.519271
6	-0.109278	4.244553	-0.357987	6	-1.329270	4.018721	-0.658680
1	0.448205	5.164785	-0.313956	1	-2.120034	4.670749	-0.987121
7	0.456844	3.027479	-0.023036	6	-0.057717	4.273816	-0.293116
6	-2.831984	1.991508	-0.761436	1	0.505066	5.190806	-0.254797
6	-3.334180	1.901575	-2.063371	7	0.496894	3.057764	0.064999
6	-4.618187	1.376634	-2.220659	6	-2.773057	2.030214	-0.773150
1	-5.038406	1.297522	-3.217525	6	-3.243098	1.970599	-2.090063
6	-5.350450	0.940041	-1.131365	6	-4.516803	1.436561	-2.293465
1	-6.340957	0.520990	-1.277467	1	-4.911337	1.379207	-3.302126
6	-4.822248	1.032948	0.148993	6	-5.272285	0.967673	-1.234797
1	-5.404328	0.681492	0.991851	1	-6.254585	0.543012	-1.415919
6	-3.561677	1.579508	0.366543	6	-4.779958	1.039484	0.060825
6	-2.562264	2.383100	-3.273792	1	-5.382298	0.664193	0.878272
1	-1.533798	2.575367	-2.960756	6	-3.530377	1.590156	0.325991
6	-2.489107	1.323388	-4.370229	6	-2.454672	2.495226	-3.272959
1	-1.963316	0.444925	-3.996311	1	-1.431440	2.681904	-2.939370
1	-1.921637	1.714955	-5.219787	6	-2.366341	1.478985	-4.409005
1	-3.481419	1.040206	-4.736053	1	-1.858093	0.578935	-4.064520
6	-3.171138	3.680890	-3.810995	1	-1.780967	1.900701	-5.231615
1	-3.215445	4.463358	-3.048064	1	-3.353162	1.219646	-4.805604
1	-4.192563	3.513574	-4.168040	6	-3.060439	3.809394	-3.774180
1	-2.579718	4.059265	-4.649951	1	-3.102640	4.571379	-2.991072
6	-3.019765	1.781878	1.768536	1	-4.082711	3.653926	-4.133679
1	-1.959583	1.511991	1.744105	1	-2.469649	4.209235	-4.603552
6	-3.690168	0.901040	2.812825	6	-3.024998	1.748815	1.747932
1	-3.661859	-0.151345	2.528460	1	-1.990224	1.394453	1.759638
1	-4.734133	1.188840	2.977472	6	-3.796186	0.910928	2.758162
1	-3.173037	1.011343	3.770553	1	-3.812780	-0.143529	2.479151
6	-3.132673	3.250531	2.190807	1	-4.828853	1.258917	2.869873
1	-2.590166	3.919203	1.520774	1	-3.321545	0.995828	3.739466
1	-2.726541	3.385747	3.198361	6	-3.043595	3.215172	2.192744
1	-4.182300	3.561724	2.205625	1	-2.414234	3.854290	1.572295
6	1.791900	2.936963	0.482912	1	-2.684345	3.296884	3.223569
6	1.997458	3.228357	1.838410	1	-4.064922	3.608763	2.161103
6	3.310008	3.229215	2.302585	6	1.846848	2.985571	0.536714
1	3.509732	3.448886	3.345368	6	2.090810	3.251654	1.891351
6	4.364755	2.942087	1.447547	6	3.419279	3.354495	2.296263
1	5.381680	2.946006	1.827465	1	3.645923	3.565490	3.335409
6	4.128023	2.644794	0.115243	6	4.455665	3.174560	1.391368
1	4.959224	2.414889	-0.541760	1	5.484404	3.257488	1.727239
6	2.832451	2.646125	-0.402263	6	4.183329	2.867871	0.068422
6	0.831567	3.474453	2.773480	1	4.999197	2.707141	-0.628086
1	-0.013048	3.818018	2.169294	6	2.869807	2.776007	-0.392421
6	0.410780	2.162199	3.436933	6	0.958224	3.438823	2.879091
1	0.188921	1.400233	2.686168	1	0.075246	2.952086	2.454482
1	-0.480410	2.309741	4.055276	6	1.243165	2.775504	4.224754
1	1.211552	1.779823	4.077313	1	1.555820	1.736826	4.105354

6	1.111228	4.553557	3.814638	1	0.343455	2.788962	4.847058
1	1.448709	5.483079	3.348137	1	2.023372	3.300670	4.784417
1	1.874565	4.239195	4.532833	6	0.634285	4.920882	3.080554
1	0.201707	4.767610	4.383285	1	0.360461	5.407281	2.142252
6	2.572000	2.412760	-1.871494	1	1.497908	5.449581	3.496813
1	1.526581	2.121773	-2.001749	1	-0.203339	5.038158	3.775028
6	3.387863	1.256794	-2.430094	6	2.579924	2.516838	-1.852259
1	3.080671	1.061425	-3.460390	1	1.517338	2.292862	-1.962629
1	3.206881	0.349431	-1.854194	6	3.314953	1.285945	-2.368585
1	4.464256	1.460322	-2.432939	1	3.010218	1.082979	-3.398372
6	2.815373	3.702468	-2.657948	1	3.059389	0.408780	-1.773504
1	2.585808	3.545871	-3.716062	1	4.402593	1.412579	-2.353370
1	3.860418	4.021833	-2.578542	6	2.898511	3.758147	-2.686757
1	2.186396	4.520787	-2.295013	1	2.638817	3.583724	-3.735014
7	1.527956	-2.762732	-0.072372	1	3.964286	4.006592	-2.637838
6	1.340965	-4.100535	0.229925	1	2.335962	4.630098	-2.339471
1	2.144086	-4.814087	0.161845	7	1.536224	-2.679063	0.100299
6	0.050857	-4.235469	0.592800	6	1.367241	-3.983051	0.531673
1	-0.523284	-5.095378	0.894055	1	2.180711	-4.688030	0.538431
7	-0.513781	-2.972663	0.510963	6	0.077270	-4.103404	0.895065
6	2.811066	-2.254664	-0.447580	1	-0.483705	-4.944206	1.263585
6	3.630235	-1.736172	0.559250	7	-0.511341	-2.864281	0.692595
6	4.908582	-1.315402	0.197102	6	2.781580	-2.233816	-0.452497
1	5.562974	-0.890974	0.951470	6	3.729809	-1.672730	0.406147
6	5.356551	-1.450977	-1.107213	6	4.967090	-1.322799	-0.132741
1	6.359246	-1.129992	-1.370431	1	5.718574	-0.874762	0.508775
6	4.526767	-1.986863	-2.080804	6	5.247987	-1.550399	-1.469147
1	4.885611	-2.076540	-3.100081	1	6.217078	-1.276554	-1.873606
6	3.227514	-2.388065	-1.777443	6	4.292603	-2.122317	-2.296252
6	3.172165	-1.653092	1.998019	1	4.521842	-2.288557	-3.342513
1	2.171150	-2.086558	2.058108	6	3.035963	-2.474833	-1.810737
6	4.081217	-2.467088	2.918074	6	3.461473	-1.491824	1.881673
1	4.135265	-3.512637	2.601677	1	2.411562	-1.727223	2.063484
1	3.703756	-2.439819	3.944874	6	4.306154	-2.464361	2.705728
1	5.100116	-2.067980	2.928215	1	4.117367	-3.501913	2.415238
6	3.064715	-0.202546	2.451176	1	4.076161	-2.361363	3.770585
1	2.394565	0.356765	1.794362	1	5.375092	-2.270028	2.571057
1	4.038665	0.293239	2.435448	6	3.681398	-0.049072	2.315854
1	2.674083	-0.148214	3.471807	1	3.061365	0.630113	1.728694
6	2.328307	-2.975755	-2.843652	1	4.723658	0.257414	2.190007
1	1.305527	-2.956605	-2.459612	1	3.423508	0.075537	3.371475
6	2.715232	-4.429122	-3.127356	6	2.018755	-3.137685	-2.714906
1	2.664361	-5.047302	-2.226949	1	1.031677	-2.974410	-2.276300
1	3.736936	-4.490154	-3.516222	6	2.271354	-4.646113	-2.790045
1	2.043131	-4.864143	-3.873235	1	2.231093	-5.116725	-1.804990
6	2.331931	-2.151038	-4.127980	1	3.256591	-4.852112	-3.221045
1	2.035419	-1.122495	-3.921411	1	1.517468	-5.126340	-3.421414
1	1.615375	-2.574310	-4.838130	6	1.988865	-2.533982	-4.115687
1	3.313479	-2.153931	-4.612826	1	1.857725	-1.452872	-4.065716
6	-1.896285	-2.746577	0.800053	1	1.148501	-2.952742	-4.676858
6	-2.797599	-2.636541	-0.265086	1	2.900158	-2.762759	-4.678004
6	-4.149041	-2.522337	0.058314	6	-1.924042	-2.680549	0.849529
1	-4.877164	-2.414643	-0.736191	6	-2.715673	-2.561037	-0.305663
6	-4.573623	-2.552426	1.376872	6	-4.093098	-2.463473	-0.130899
1	-5.632577	-2.480101	1.603909	1	-4.727782	-2.340599	-0.999853
6	-3.655012	-2.663149	2.411035	6	-4.666051	-2.537466	1.129647

1	-4.003733	-2.673978	3.437046	1	-5.744108	-2.475424	1.238850
6	-2.290491	-2.745950	2.144345	6	-3.865739	-2.694284	2.247551
6	-2.325542	-2.692326	-1.702914	1	-4.321356	-2.758670	3.230086
1	-1.364110	-2.172704	-1.759879	6	-2.476460	-2.755768	2.134488
6	-2.117029	-4.143246	-2.147490	6	-2.117663	-2.636459	-1.694250
1	-1.384348	-4.663339	-1.526407	1	-1.145217	-2.141029	-1.676984
1	-1.755367	-4.168363	-3.179893	6	-1.901249	-4.099229	-2.093262
1	-3.058790	-4.700757	-2.103536	1	-1.247498	-4.622055	-1.390464
6	-3.258931	-1.974307	-2.667045	1	-1.437661	-4.152442	-3.083254
1	-3.458704	-0.953690	-2.338568	1	-2.855021	-4.636089	-2.134132
1	-4.214854	-2.497109	-2.784835	6	-2.935451	-1.905809	-2.749029
1	-2.790847	-1.922456	-3.653060	1	-3.143647	-0.879287	-2.444099
6	-1.257399	-2.776167	3.253513	1	-3.885914	-2.407509	-2.962770
1	-0.447854	-3.442052	2.935978	1	-2.366351	-1.867354	-3.680987
6	-1.793552	-3.315246	4.574495	6	-1.637509	-2.939423	3.382669
1	-2.265417	-4.294323	4.452760	1	-0.590145	-2.788726	3.110954
1	-2.526924	-2.636151	5.020441	6	-1.789800	-4.357284	3.939113
1	-0.974340	-3.418876	5.291093	1	-1.510850	-5.119515	3.207591
6	-0.651594	-1.382438	3.443454	1	-2.827175	-4.547940	4.231333
1	-0.245156	-0.991206	2.506609	1	-1.160039	-4.491334	4.823670
1	0.154764	-1.410744	4.183216	6	-1.979252	-1.915914	4.465051
1	-1.412784	-0.680915	3.796485	1	-1.921783	-0.897492	4.081406
				1	-1.279057	-2.007291	5.300228
				1	-2.987383	-2.071111	4.861417

End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 177° (OST) | **End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 172° (OST)**

46	-0.005640	0.019208	0.023368	46	-0.005527	0.012531	-0.068792
8	-0.136304	0.073148	-2.202735	8	-0.129100	0.073482	-2.272049
8	-0.055391	-1.012052	-2.847626	8	-0.065435	-1.013337	-2.915753
6	0.373446	-1.989360	0.182940	6	0.398736	-1.986453	0.162321
7	1.517224	-2.676734	-0.104578	7	1.557318	-2.658260	-0.105053
6	1.338036	-4.046438	-0.004545	6	1.403231	-4.028888	0.016840
1	2.139757	-4.740630	-0.187421	1	2.219109	-4.710985	-0.147990
6	0.056065	-4.240735	0.358934	6	0.122411	-4.240663	0.374349
1	-0.506937	-5.138231	0.551027	1	-0.425706	-5.145086	0.577084
7	-0.509300	-2.982622	0.476673	7	-0.467576	-2.991465	0.466930
6	2.798075	-2.107823	-0.391906	6	2.829310	-2.070245	-0.394762
6	3.354826	-2.308164	-1.660291	6	3.380295	-2.248875	-1.668537
6	4.650414	-1.836455	-1.877711	6	4.670555	-1.762783	-1.886457
1	5.108752	-1.979415	-2.850354	1	5.125502	-1.888873	-2.863008
6	5.342308	-1.168865	-0.883900	6	5.362324	-1.102957	-0.886918
1	6.342015	-0.793411	-1.077721	1	6.358059	-0.717097	-1.080873
6	4.761100	-0.973766	0.361986	6	4.785680	-0.927924	0.364034
1	5.312484	-0.444681	1.129288	1	5.336190	-0.402923	1.134900
6	3.488526	-1.458697	0.646067	6	3.518132	-1.426551	0.647177
6	2.620642	-3.027854	-2.773358	6	2.644354	-2.961514	-2.784411
1	1.580792	-3.155218	-2.463863	1	1.603117	-3.082719	-2.476711
6	2.597443	-2.219364	-4.069393	6	2.629480	-2.149812	-4.078443
1	2.095526	-1.263904	-3.920121	1	2.150103	-1.183565	-3.924869
1	2.042643	-2.769468	-4.835145	1	2.056869	-2.685521	-4.840995
1	3.605866	-2.040042	-4.455630	1	3.638802	-1.992120	-4.471906
6	3.236038	-4.407933	-3.019092	6	3.251601	-4.344607	-3.032926
1	3.254603	-5.020283	-2.113425	1	3.255741	-4.962768	-2.131266
1	4.268529	-4.315864	-3.371702	1	4.288071	-4.257767	-3.375241
1	2.667899	-4.948468	-3.781974	1	2.686398	-4.875762	-3.804499
6	2.892531	-1.348219	2.035536	6	2.923036	-1.333097	2.038134

1	1.842595	-1.061520	1.908099	1	1.868213	-1.064547	1.912666
6	3.548323	-0.279196	2.895499	6	3.563561	-0.257473	2.901307
1	3.545170	0.692198	2.400243	1	3.543959	0.715936	2.410739
1	4.581558	-0.537995	3.151765	1	4.601429	-0.501410	3.153290
1	2.998852	-0.182541	3.836086	1	3.015900	-0.174483	3.844266
6	2.945892	-2.696810	2.760170	6	3.001530	-2.682400	2.759244
1	2.418034	-3.483427	2.218189	1	2.486078	-3.476973	2.217378
1	2.489337	-2.609522	3.751307	1	2.546082	-2.605142	3.751751
1	3.984784	-3.016180	2.894676	1	4.046292	-2.983418	2.890587
6	-1.868874	-2.822081	0.888204	6	-1.832647	-2.855410	0.869698
6	-2.150071	-2.833294	2.261696	6	-2.120418	-2.889453	2.242035
6	-3.489290	-2.822494	2.640463	6	-3.460965	-2.912785	2.614486
1	-3.748963	-2.838051	3.693062	1	-3.725294	-2.948650	3.665276
6	-4.499257	-2.781784	1.687244	6	-4.467260	-2.879367	1.656738
1	-5.537440	-2.771902	2.003916	1	-5.506859	-2.895932	1.968336
6	-4.188175	-2.744166	0.338497	6	-4.150591	-2.813913	0.310671
1	-4.983289	-2.701766	-0.398263	1	-4.942804	-2.776101	-0.429493
6	-2.861533	-2.776659	-0.091615	6	-2.821285	-2.813839	-0.113924
6	-1.035563	-2.800108	3.286125	6	-1.009600	-2.840718	3.270134
1	-0.150087	-3.250846	2.827863	1	-0.122965	-3.300790	2.823143
6	-0.686770	-1.347497	3.619424	6	-0.659494	-1.382522	3.578045
1	-0.451054	-0.784988	2.709593	1	-0.422985	-0.834846	2.659801
1	0.177337	-1.299854	4.289926	1	0.203989	-1.324188	4.248509
1	-1.529980	-0.854164	4.112622	1	-1.502699	-0.880754	4.062459
6	-1.349588	-3.594993	4.549006	6	-1.327786	-3.610748	4.546877
1	-1.645937	-4.621282	4.315158	1	-1.627101	-4.640411	4.332410
1	-2.153613	-3.133559	5.130368	1	-2.130664	-3.135469	5.118668
1	-0.466989	-3.632874	5.193817	1	-0.446018	-3.639164	5.193221
6	-2.525051	-2.799497	-1.563649	6	-2.480645	-2.806016	-1.585024
1	-1.446657	-2.666007	-1.671545	1	-1.403717	-2.658945	-1.689046
6	-3.176068	-1.635128	-2.297610	6	-3.144020	-1.634572	-2.297364
1	-2.849622	-1.623250	-3.340455	1	-2.817039	-1.599347	-3.339446
1	-2.880262	-0.689046	-1.842650	1	-2.858998	-0.693613	-1.824608
1	-4.268827	-1.697106	-2.282267	1	-4.235994	-1.709002	-2.283456
6	-2.904176	-4.144755	-2.183387	6	-2.843640	-4.143233	-2.231034
1	-2.620381	-4.167180	-3.239629	1	-2.555929	-4.142565	-3.286389
1	-3.983324	-4.320031	-2.119063	1	-3.921034	-4.331317	-2.174059
1	-2.400366	-4.974510	-1.678707	1	-2.332461	-4.976692	-1.739963
6	-0.383171	2.033521	-0.017730	6	-0.405961	2.023299	-0.002612
7	-1.527391	2.667113	-0.401240	7	-1.566489	2.657454	-0.334803
6	-1.360509	4.039581	-0.482652	6	-1.422712	4.034724	-0.349937
1	-2.166786	4.695552	-0.762466	1	-2.243626	4.690465	-0.584576
6	-0.081802	4.290844	-0.141247	6	-0.142689	4.289255	-0.016473
1	0.473288	5.210909	-0.069541	1	0.398982	5.213663	0.092440
7	0.492591	3.064019	0.144303	7	0.456617	3.059175	0.196273
6	-2.785685	2.047131	-0.681517	6	-2.815505	2.029879	-0.639202
6	-3.555839	1.574283	0.393077	6	-3.589221	1.528639	0.419102
6	-4.813006	1.056909	0.095911	6	-4.837753	1.002393	0.101591
1	-5.428543	0.658883	0.893137	1	-5.455423	0.582361	0.885776
6	-5.296359	1.051170	-1.205826	6	-5.308435	1.014304	-1.204611
1	-6.286526	0.656896	-1.410815	1	-6.291713	0.611925	-1.426167
6	-4.517589	1.532482	-2.242555	6	-4.525833	1.522674	-2.225721
1	-4.897709	1.507345	-3.258247	1	-4.896325	1.510724	-3.245139
6	-3.234030	2.025521	-2.006345	6	-3.250640	2.026823	-1.968652
6	-3.048183	1.665793	1.819225	6	-3.094029	1.600281	1.850482
1	-2.000649	1.343793	1.801920	1	-2.037052	1.311634	1.834395

6	-3.101377	3.106163	2.338526	6	-3.197433	3.025010	2.404215
1	-2.504086	3.791543	1.735237	1	-2.620273	3.743580	1.820426
1	-2.720737	3.147669	3.363899	1	-2.822953	3.054536	3.432308
1	-4.133823	3.471140	2.347248	1	-4.241638	3.354714	2.415858
6	-3.788504	0.750858	2.783105	6	-3.814378	0.640026	2.784876
1	-3.789753	-0.282945	2.436333	1	-3.785572	-0.383401	2.410571
1	-4.825423	1.071459	2.932227	1	-4.860612	0.928195	2.934536
1	-3.299581	0.779736	3.760897	1	-3.333763	0.656225	3.767105
6	-2.391614	2.528349	-3.161215	6	-2.400874	2.562463	-3.103024
1	-1.382945	2.715759	-2.784600	1	-1.391924	2.727644	-2.716029
6	-2.956056	3.842032	-3.707228	6	-2.951935	3.899615	-3.603748
1	-3.027280	4.611151	-2.933265	1	-3.012043	4.643142	-2.804397
1	-3.960387	3.693034	-4.116459	1	-3.958738	3.774856	-4.015178
1	-2.319914	4.226743	-4.509877	1	-2.312946	4.303823	-4.394529
6	-2.262505	1.492995	-4.277443	6	-2.277461	1.566695	-4.255034
1	-1.797342	0.577587	-3.912529	1	-1.837341	0.628401	-3.918301
1	-1.633398	1.893932	-5.078091	1	-1.627850	1.982772	-5.031127
1	-3.234808	1.246986	-4.715911	1	-3.248074	1.359071	-4.716616
6	1.870295	2.946776	0.505896	6	1.840482	2.949284	0.535649
6	2.794830	2.627635	-0.491945	6	2.755099	2.647652	-0.477522
6	4.141925	2.609186	-0.132093	6	4.106473	2.638613	-0.134359
1	4.886862	2.350140	-0.875621	1	4.844436	2.390506	-0.888188
6	4.538195	2.926133	1.157131	6	4.516464	2.950792	1.152052
1	5.592635	2.919980	1.414458	1	5.574281	2.953376	1.395275
6	3.595713	3.243332	2.126641	6	3.584027	3.250663	2.136258
1	3.922647	3.477678	3.133096	1	3.921692	3.480578	3.140115
6	2.236552	3.247618	1.824237	6	2.220787	3.241336	1.851899
6	2.355278	2.384033	-1.918366	6	2.294383	2.413155	-1.899028
1	1.308084	2.074371	-1.899667	1	1.281204	2.006437	-1.858606
6	2.460186	3.678302	-2.728585	6	2.249961	3.738619	-2.663853
1	1.861369	4.479921	-2.287391	1	1.590375	4.463563	-2.179537
1	2.104467	3.514795	-3.750366	1	1.880498	3.574787	-3.680738
1	3.498587	4.022594	-2.780211	1	3.249399	4.181428	-2.730950
6	3.118331	1.249409	-2.583892	6	3.136603	1.383113	-2.635362
1	3.042398	0.337451	-1.991991	1	3.191118	0.451716	-2.071291
1	4.178659	1.483017	-2.725496	1	4.156594	1.734714	-2.824081
1	2.690182	1.048475	-3.569137	1	2.680305	1.164876	-3.604143
6	1.180100	3.502623	2.879343	6	1.174656	3.473553	2.923114
1	0.339889	4.008906	2.392750	1	0.335023	4.001972	2.459613
6	1.655945	4.399339	4.016122	6	1.666151	4.331586	4.082596
1	2.076069	5.337797	3.643479	1	2.090735	5.277873	3.735592
1	2.416264	3.905565	4.629148	1	2.427065	3.813808	4.674859
1	0.817432	4.639344	4.675641	1	0.834423	4.558018	4.755321
6	0.654876	2.168664	3.417418	6	0.639953	2.129501	3.426388
1	0.319252	1.519379	2.603626	1	0.291067	1.505887	2.598492
1	-0.184609	2.331208	4.100779	1	-0.192509	2.281356	4.120816
1	1.443087	1.641194	3.962625	1	1.426567	1.579072	3.950589
End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 167° (OST)				**End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 162° (OST)**			
46	-0.014901	0.010608	-0.165327	46	0.064417	-0.039000	-0.262079
8	-0.123346	0.126547	-2.353134	8	0.126418	-0.351351	-2.427681
8	-0.114162	-0.948680	-3.016523	8	0.428988	0.626703	-3.166370
6	0.371444	-1.989751	0.099623	6	-0.361675	1.972314	-0.172556
7	1.532004	-2.663227	-0.158016	7	-1.525462	2.572117	-0.565246
6	1.373855	-4.034153	-0.048833	6	-1.403743	3.948679	-0.639273
1	2.190494	-4.716874	-0.207859	1	-2.225816	4.579911	-0.929997

6	0.088988	-4.245598	0.294488	6	-0.141047	4.241710	-0.272648
1	-0.462655	-5.150353	0.486132	1	0.378791	5.180295	-0.179834
7	-0.500025	-2.996078	0.390247	7	0.472011	3.034977	0.017816
6	2.807200	-2.074677	-0.433975	6	-2.778494	1.915586	-0.787783
6	3.340961	-2.197019	-1.721438	6	-3.239349	1.764977	-2.099082
6	4.633980	-1.715075	-1.931086	6	-4.517596	1.233123	-2.275340
1	5.077032	-1.799264	-2.917447	1	-4.906015	1.108968	-3.280348
6	5.344429	-1.112109	-0.908791	6	-5.284484	0.845097	-1.190678
1	6.342375	-0.728518	-1.095715	1	-6.270812	0.420637	-1.349080
6	4.783486	-0.989533	0.355174	6	-4.793982	0.988681	0.099736
1	5.347439	-0.504358	1.142060	1	-5.399433	0.667380	0.938255
6	3.512749	-1.485734	0.628672	6	-3.539998	1.544730	0.332833
6	2.581033	-2.847689	-2.858503	6	-2.414808	2.181577	-3.297714
1	1.533953	-2.930915	-2.557185	1	-1.382481	2.313568	-2.964800
6	2.607403	-2.004211	-4.131710	6	-2.393351	1.110132	-4.385969
1	2.191600	-1.013283	-3.952346	1	-2.046390	0.156650	-3.988296
1	1.996334	-2.483526	-4.901643	1	-1.703165	1.406953	-5.179731
1	3.621523	-1.900406	-4.530831	1	-3.381048	0.968375	-4.837173
6	3.129344	-4.248571	-3.142371	6	-2.921426	3.508842	-3.867018
1	3.094297	-4.892825	-2.260184	1	-2.897994	4.309264	-3.123223
1	4.172548	-4.196907	-3.471280	1	-3.954236	3.411744	-4.217741
1	2.549886	-4.730771	-3.935286	1	-2.304178	3.819162	-4.715330
6	2.928211	-1.436447	2.026878	6	-3.032319	1.785049	1.740902
1	1.879762	-1.137041	1.919223	1	-1.963571	1.547950	1.737327
6	3.604350	-0.414747	2.928284	6	-3.693282	0.892034	2.780528
1	3.611627	0.577910	2.477532	1	-3.623533	-0.161010	2.507817
1	4.635778	-0.700054	3.162351	1	-4.749509	1.145629	2.921602
1	3.066071	-0.354668	3.878315	1	-3.200876	1.029664	3.747650
6	2.977069	-2.813228	2.697282	6	-3.204922	3.251631	2.149147
1	2.430559	-3.572820	2.136818	1	-2.680310	3.935692	1.480995
1	2.538345	-2.757937	3.698697	1	-2.815136	3.408445	3.160194
1	4.014376	-3.148237	2.802282	1	-4.265685	3.523107	2.151053
6	-1.866662	-2.864163	0.789633	6	1.800817	3.000779	0.546492
6	-2.159748	-2.951733	2.159048	6	1.966696	3.288016	1.910164
6	-3.501208	-2.984170	2.526685	6	3.267873	3.380085	2.394504
1	-3.768783	-3.060808	3.574389	1	3.435316	3.601489	3.442476
6	-4.504409	-2.906400	1.568107	6	4.355393	3.188452	1.552855
1	-5.545077	-2.930114	1.875604	1	5.362974	3.268145	1.948672
6	-4.182864	-2.787889	0.227030	6	4.160279	2.888107	0.215706
1	-4.972508	-2.716482	-0.513382	1	5.015506	2.732050	-0.433327
6	-2.852135	-2.778893	-0.194036	6	2.874919	2.795368	-0.320223
6	-1.050994	-2.946751	3.190954	6	0.771549	3.426139	2.830044
1	-0.173073	-3.418121	2.738342	1	-0.076786	3.764267	2.227637
6	-0.670065	-1.501967	3.524351	6	0.404472	2.055350	3.400273
1	-0.425319	-0.942772	2.615923	1	0.251307	1.329651	2.597205
1	0.195823	-1.473566	4.193534	1	-0.512888	2.116521	3.994589
1	-1.501741	-0.992241	4.020117	1	1.204619	1.679566	4.045608
6	-1.388412	-3.731112	4.453653	6	0.973460	4.450035	3.941621
1	-1.710040	-4.750206	4.221555	1	1.275824	5.422611	3.543587
1	-2.181464	-3.247731	5.032408	1	1.732497	4.126978	4.660587
1	-0.508475	-3.789826	5.100373	1	0.040659	4.583682	4.496812
6	-2.509719	-2.721602	-1.663527	6	2.672011	2.518933	-1.790413
1	-1.430971	-2.584337	-1.762077	1	1.606497	2.364493	-1.970014
6	-3.159162	-1.518260	-2.334972	6	3.366658	1.229036	-2.207880
1	-2.835935	-1.455258	-3.376871	1	3.144270	1.007566	-3.254504
1	-2.858182	-0.596225	-1.835000	1	3.006790	0.391938	-1.607011

1	-4.252064	-1.577225	-2.318300	1	4.453489	1.291629	-2.094054
6	-2.887545	-4.030688	-2.357135	6	3.130263	3.709329	-2.632828
1	-2.597500	-3.995395	-3.411301	1	2.939766	3.515836	-3.692441
1	-3.967190	-4.208114	-2.308883	1	4.202836	3.894179	-2.510076
1	-2.386928	-4.887106	-1.895559	1	2.599554	4.624433	-2.353404
6	-0.377909	2.019330	0.045201	6	0.389324	-1.996270	0.293744
7	-1.538968	2.689724	-0.206365	7	1.546379	-2.712028	0.204429
6	-1.381736	4.061877	-0.113536	6	1.408270	-4.000949	0.687674
1	-2.200000	4.742162	-0.276083	1	2.231606	-4.694636	0.706764
6	-0.091905	4.277426	0.208314	6	0.124889	-4.124562	1.076748
1	0.461218	5.185664	0.378863	1	-0.420849	-4.957082	1.487937
7	0.500841	3.029063	0.304333	7	-0.480830	-2.902660	0.828251
6	-2.795943	2.097157	-0.545451	6	2.789516	-2.240479	-0.321170
6	-3.585727	1.568722	0.486218	6	3.721910	-1.709031	0.572598
6	-4.840699	1.076484	0.140269	6	4.969622	-1.348055	0.066414
1	-5.471702	0.638770	0.904068	1	5.711508	-0.920379	0.732784
6	-5.298545	1.143237	-1.168721	6	5.270921	-1.534787	-1.272523
1	-6.286205	0.765627	-1.413328	1	6.249364	-1.256550	-1.650722
6	-4.497490	1.673422	-2.164762	6	4.322064	-2.058834	-2.138989
1	-4.858311	1.702988	-3.187099	1	4.564418	-2.176587	-3.188800
6	-3.217201	2.147312	-1.878285	6	3.054758	-2.416478	-1.686383
6	-3.097344	1.573006	1.921394	6	3.402480	-1.523843	2.038971
1	-2.035772	1.303475	1.894776	1	2.393663	-1.905604	2.213770
6	-3.227632	2.964232	2.549221	6	4.359661	-2.319016	2.925682
1	-2.659184	3.721523	2.007318	1	4.347682	-3.383064	2.672586
1	-2.859037	2.945721	3.579712	1	4.077903	-2.215215	3.977912
1	-4.277274	3.275520	2.571497	1	5.389253	-1.962940	2.821097
6	-3.805263	0.550782	2.797664	6	3.394460	-0.043332	2.402083
1	-3.760823	-0.448326	2.364095	1	2.692826	0.506030	1.770166
1	-4.855999	0.814240	2.960314	1	4.383086	0.405043	2.271569
1	-3.327568	0.516989	3.780833	1	3.098155	0.093746	3.446613
6	-2.343089	2.710533	-2.980051	6	2.019681	-3.001452	-2.623917
1	-1.327010	2.798475	-2.586084	1	1.036516	-2.780236	-2.200177
6	-2.825289	4.103973	-3.390285	6	2.176760	-4.521692	-2.717303
1	-2.840853	4.796392	-2.544698	1	2.082635	-5.002287	-1.740684
1	-3.839615	4.057900	-3.799825	1	3.156825	-4.782796	-3.130206
1	-2.169759	4.524184	-4.158918	1	1.408893	-4.943588	-3.372947
6	-2.270874	1.788531	-4.195614	6	2.052143	-2.376202	-4.014900
1	-1.896880	0.802493	-3.920857	1	1.959649	-1.290552	-3.965784
1	-1.585938	2.212048	-4.936345	1	1.209999	-2.753603	-4.601946
1	-3.246873	1.677469	-4.678867	1	2.966943	-2.634895	-4.558313
6	1.888480	2.883952	0.614040	6	-1.879234	-2.710981	1.057651
6	2.785620	2.618248	-0.425609	6	-2.743264	-2.657095	-0.043734
6	4.140909	2.576916	-0.101770	6	-4.108880	-2.578032	0.224287
1	4.865526	2.352661	-0.875368	1	-4.808218	-2.510777	-0.599722
6	4.572881	2.826652	1.191319	6	-4.585868	-2.595794	1.525244
1	5.634036	2.806058	1.418706	1	-5.654765	-2.552496	1.708434
6	3.658486	3.092571	2.201209	6	-3.706014	-2.657274	2.595767
1	4.012622	3.273207	3.209504	1	-4.093992	-2.657541	3.607355
6	2.291063	3.110390	1.936660	6	-2.329355	-2.697103	2.385202
6	2.299645	2.449655	-1.848746	6	-2.215365	-2.732543	-1.462271
1	1.317537	1.972221	-1.807702	1	-1.318917	-2.106735	-1.506390
6	2.142751	3.815586	-2.522824	6	-1.818168	-4.167264	-1.823454
1	1.448673	4.461241	-1.979192	1	-1.051121	-4.567158	-1.157115
1	1.757335	3.690747	-3.539343	1	-1.421058	-4.197849	-2.842717
1	3.107905	4.329573	-2.584723	1	-2.688720	-4.830387	-1.778831

6	3.185750	1.536419	-2.681665	6	-3.185635	-2.184581	-2.498129
1	3.329835	0.574127	-2.189322	1	-3.512478	-1.174716	-2.245080
1	4.169080	1.977289	-2.879004	1	-4.070455	-2.821344	-2.609524
1	2.710176	1.353475	-3.648509	1	-2.689619	-2.144175	-3.471081
6	1.264085	3.304888	3.034290	6	-1.343359	-2.670323	3.538154
1	0.429414	3.874621	2.613016	1	-0.534825	-3.370602	3.304146
6	1.788548	4.089758	4.230585	6	-1.942797	-3.106462	4.869401
1	2.229865	5.043736	3.928314	1	-2.423269	-4.086601	4.800358
1	2.544645	3.525639	4.785692	1	-2.683734	-2.387413	5.233018
1	0.970061	4.298643	4.924882	1	-1.155550	-3.167017	5.625661
6	0.706742	1.947956	3.474420	6	-0.713042	-1.280647	3.660913
1	0.334247	1.374159	2.621422	1	-0.285080	-0.946518	2.712595
1	-0.113493	2.081853	4.186929	1	0.079389	-1.283539	4.416045
1	1.487400	1.355450	3.959903	1	-1.465962	-0.547287	3.961843

End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 157° (OST) ‖ **End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 152° (OST)**

46	0.062738	-0.085366	-0.338061	46	0.069466	-0.115921	-0.415659
8	0.125764	-0.606724	-2.448953	8	0.122639	-0.727649	-2.487499
8	0.475347	0.282232	-3.271438	8	0.492599	0.124258	-3.337219
6	-0.384407	1.933276	-0.338100	6	-0.390634	1.911725	-0.395966
7	-1.554092	2.493793	-0.772218	7	-1.568355	2.461612	-0.824656
6	-1.444415	3.860921	-0.951277	6	-1.469265	3.827015	-1.020022
1	-2.270789	4.461306	-1.290872	1	-2.301502	4.418787	-1.360332
6	-0.184969	4.192156	-0.606157	6	-0.209439	4.170312	-0.688955
1	0.326363	5.139856	-0.585612	1	0.295519	5.121713	-0.684256
7	0.438913	3.017242	-0.222905	7	0.425867	3.004274	-0.297158
6	-2.796767	1.803310	-0.948002	6	-2.805023	1.758668	-0.996254
6	-3.221028	1.487161	-2.242265	6	-3.202200	1.387652	-2.284953
6	-4.481721	0.904763	-2.381483	6	-4.454413	0.787857	-2.424144
1	-4.841897	0.651680	-3.372539	1	-4.792416	0.489854	-3.410320
6	-5.268181	0.632888	-1.275582	6	-5.260604	0.555313	-1.323400
1	-6.240884	0.168751	-1.404182	1	-6.226496	0.077009	-1.451540
6	-4.815808	0.945056	-0.001388	6	-4.836451	0.924019	-0.055037
1	-5.436025	0.713696	0.855702	1	-5.471769	0.721973	0.798330
6	-3.577667	1.549918	0.191413	6	-3.605937	1.545213	0.137155
6	-2.377418	1.788796	-3.461735	6	-2.337525	1.651427	-3.498596
1	-1.346967	1.935124	-3.128496	1	-1.307062	1.772776	-3.155017
6	-2.360467	0.633556	-4.459970	6	-2.342264	0.488386	-4.487430
1	-2.051868	-0.294925	-3.979907	1	-2.079362	-0.448106	-3.995599
1	-1.641866	0.846472	-5.255182	1	-1.598999	0.668680	-5.267697
1	-3.340000	0.484003	-4.926092	1	-3.316005	0.372479	-4.974864
6	-2.858173	3.071731	-4.144841	6	-2.774146	2.939960	-4.201024
1	-2.823384	3.932394	-3.472482	1	-2.717487	3.807507	-3.539659
1	-3.891050	2.961553	-4.491639	1	-3.807136	2.855655	-4.554792
1	-2.231819	3.298106	-5.012869	1	-2.134143	3.135550	-5.066539
6	-3.104887	1.955975	1.573325	6	-3.161047	2.002058	1.512949
1	-2.032400	1.740819	1.615774	1	-2.088987	1.790987	1.584231
6	-3.774556	1.172928	2.693568	6	-3.854990	1.258981	2.646138
1	-3.688864	0.097502	2.538236	1	-3.770301	0.178546	2.530268
1	-4.835862	1.427284	2.786967	1	-4.916991	1.519550	2.708423
1	-3.301951	1.422210	3.648189	1	-3.401863	1.540656	3.601198
6	-3.310632	3.454852	1.815705	6	-3.373721	3.507667	1.703053
1	-2.780030	4.072025	1.090096	1	-2.816888	4.104131	0.980279
1	-2.948841	3.727181	2.812476	1	-3.047255	3.808667	2.703768
1	-4.375323	3.705312	1.763488	1	-4.435740	3.756282	1.606591
6	1.768021	3.037042	0.307496	6	1.762944	3.043563	0.212719

6	1.934759	3.474570	1.631077	6	1.950432	3.549649	1.509772
6	3.235975	3.600193	2.108281	6	3.258730	3.694258	1.961435
1	3.403918	3.935242	3.125459	1	3.442635	4.082515	2.956477
6	4.323730	3.300902	1.298523	6	4.333946	3.345394	1.154511
1	5.331186	3.407580	1.688161	1	5.347102	3.466996	1.524360
6	4.127541	2.864690	-0.000682	6	4.117719	2.842156	-0.116673
1	4.982257	2.631571	-0.626572	1	4.962571	2.571963	-0.740810
6	2.842372	2.731485	-0.528918	6	2.824845	2.688393	-0.620384
6	0.741214	3.755038	2.521495	6	0.769463	3.879590	2.401096
1	-0.089237	4.063104	1.879477	1	-0.050934	4.216384	1.760060
6	0.310883	2.472926	3.233628	6	0.291073	2.617049	3.117663
1	0.113559	1.674596	2.514909	1	0.078514	1.819042	2.403265
1	-0.596553	2.643554	3.821841	1	-0.617618	2.820189	3.693391
1	1.097745	2.128044	3.911337	1	1.058760	2.254214	3.807646
6	0.981536	4.882935	3.519597	6	1.050694	4.999471	3.396843
1	1.338524	5.790240	3.024509	1	1.442391	5.892258	2.901518
1	1.714092	4.602320	4.282440	1	1.770120	4.692156	4.161999
1	0.050159	5.122291	4.040608	1	0.127892	5.274382	3.915423
6	2.645668	2.312857	-1.965790	6	2.608453	2.202875	-2.033188
1	1.583125	2.127260	-2.131646	1	1.547488	1.985564	-2.167221
6	3.362208	1.001146	-2.257122	6	3.349585	0.897361	-2.288249
1	3.132128	0.666446	-3.271191	1	3.100978	0.516150	-3.281143
1	3.026611	0.226134	-1.565775	1	3.050214	0.144600	-1.556783
1	4.448868	1.095831	-2.165460	1	4.435849	1.019463	-2.230445
6	3.086205	3.425816	-2.916770	6	2.999643	3.285406	-3.039442
1	2.903321	3.128378	-3.953435	1	2.799817	2.940186	-4.058003
1	4.154786	3.640877	-2.809307	1	4.064898	3.529635	-2.966556
1	2.537554	4.353470	-2.727681	1	2.432792	4.206945	-2.875916
6	0.428335	-1.949957	0.479357	6	0.434804	-1.913663	0.549335
7	1.603061	-2.644106	0.517178	7	1.617268	-2.589026	0.658153
6	1.473957	-3.861368	1.164113	6	1.488978	-3.759728	1.386877
1	2.307830	-4.531188	1.289846	1	2.326666	-4.410722	1.572656
6	0.183732	-3.959999	1.535862	6	0.193430	-3.847521	1.741550
1	-0.356025	-4.742912	2.041594	1	-0.347019	-4.599423	2.291537
7	-0.438247	-2.795763	1.111336	7	-0.433829	-2.723145	1.225817
6	2.841797	-2.246832	-0.079296	6	2.856909	-2.231824	0.037148
6	3.808547	-1.653291	0.740512	6	3.830139	-1.599680	0.820837
6	5.042215	-1.352867	0.167782	6	5.063222	-1.336217	0.229284
1	5.811155	-0.882914	0.769858	1	5.836812	-0.840192	0.803612
6	5.300746	-1.657651	-1.159904	6	5.315695	-1.711128	-1.081622
1	6.269731	-1.422556	-1.588426	1	6.283815	-1.502244	-1.525351
6	4.326544	-2.251812	-1.946542	6	4.337314	-2.344327	-1.831077
1	4.538415	-2.472365	-2.986141	1	4.545570	-2.623278	-2.857203
6	3.070523	-2.557417	-1.425975	6	3.082338	-2.618979	-1.290131
6	3.500560	-1.322592	2.184622	6	3.527140	-1.196012	2.247543
1	2.767996	-2.054439	2.540949	1	2.844206	-1.944976	2.662998
6	4.718656	-1.417701	3.097777	6	4.761043	-1.158344	3.142660
1	5.224392	-2.382840	3.002007	1	5.326952	-2.093366	3.098446
1	4.410238	-1.294984	4.139839	1	4.459114	-0.990421	4.180230
1	5.446771	-0.629228	2.884060	1	5.432370	-0.338839	2.867942
6	2.855467	0.058722	2.276458	6	2.805616	0.150000	2.266614
1	1.964488	0.125912	1.643190	1	1.905883	0.133135	1.643428
1	3.553529	0.830460	1.944096	1	3.458355	0.935361	1.879590
1	2.565647	0.278122	3.308568	1	2.516934	0.414974	3.288140
6	2.016587	-3.239158	-2.272978	6	2.030112	-3.353777	-2.093328
1	1.041629	-2.945037	-1.876261	1	1.054092	-3.033367	-1.720751

6	2.146511	-4.761305	-2.163946	6	2.159268	-4.864923	-1.879752
1	2.038578	-5.107106	-1.133383	1	2.046925	-5.138659	-0.828222
1	3.123628	-5.090859	-2.532188	1	3.138192	-5.218549	-2.219906
1	1.374222	-5.252452	-2.763619	1	1.389736	-5.396640	-2.447490
6	2.051005	-2.808017	-3.735673	6	2.069923	-3.024373	-3.581835
1	2.002175	-1.722916	-3.834740	1	2.024553	-1.948537	-3.755720
1	1.185949	-3.226483	-4.257711	1	1.205599	-3.475971	-4.076705
1	2.946852	-3.175156	-4.247512	1	2.966378	-3.427665	-4.064584
6	-1.844758	-2.602805	1.283651	6	-1.845339	-2.538860	1.364110
6	-2.684487	-2.701074	0.166474	6	-2.666727	-2.709025	0.242006
6	-4.056746	-2.610038	0.392128	6	-4.043769	-2.630838	0.442079
1	-4.737193	-2.659545	-0.448810	1	-4.709794	-2.735914	-0.405353
6	-4.564277	-2.470007	1.673632	6	-4.573784	-2.436407	1.706955
1	-5.637652	-2.420957	1.826721	1	-5.650096	-2.400339	1.841991
6	-3.708931	-2.382748	2.761910	6	-3.736672	-2.278583	2.801479
1	-4.121216	-2.263569	3.756772	1	-4.166493	-2.117832	3.782938
6	-2.327325	-2.427723	2.588468	6	-2.351985	-2.305040	2.650842
6	-2.126642	-2.949409	-1.220063	6	-2.085315	-3.022993	-1.120748
1	-1.231581	-2.329206	-1.322397	1	-1.187229	-2.409675	-1.235228
6	-1.719204	-4.416100	-1.387495	6	-1.677464	-4.496301	-1.208352
1	-0.964497	-4.721501	-0.659825	1	-0.937139	-4.765285	-0.451675
1	-1.302809	-4.576678	-2.386608	1	-1.242182	-4.706758	-2.190032
1	-2.588532	-5.072309	-1.272881	1	-2.549527	-5.145818	-1.077544
6	-3.074570	-2.538102	-2.337094	6	-3.011843	-2.661659	-2.272611
1	-3.414620	-1.508560	-2.212729	1	-3.354148	-1.627810	-2.198099
1	-3.951979	-3.192009	-2.394230	1	-3.888399	-3.317582	-2.318819
1	-2.553799	-2.607767	-3.295480	1	-2.472524	-2.771784	-3.216890
6	-1.370056	-2.242418	3.750787	6	-1.417512	-2.039596	3.816259
1	-0.554245	-2.962335	3.630997	1	-0.596867	-2.761830	3.759504
6	-1.999711	-2.501961	5.113655	6	-2.071242	-2.212318	5.181411
1	-2.476251	-3.485236	5.163468	1	-2.540019	-3.194741	5.288906
1	-2.750605	-1.745257	5.362176	1	-2.833766	-1.448288	5.363621
1	-1.230344	-2.458432	5.889282	1	-1.317564	-2.108877	5.966662
6	-0.745789	-0.845668	3.702358	6	-0.797502	-0.646151	3.687093
1	-0.301249	-0.636586	2.726362	1	-0.341891	-0.497169	2.705428
1	0.033673	-0.746311	4.464272	1	-0.028055	-0.495287	4.450585
1	-1.505361	-0.083019	3.892690	1	-1.561903	0.123607	3.819160

End-on [Pd(IPr)$_2$(η^1-O$_2$)] scan C-Pd-C = 147° (OST) | | | | **End-on [Pd(IPr)$_2$(η^1-O$_2$)] scan C-Pd-C = 142° (OST)** | | | |

46	0.094801	-0.167512	-0.496577	46	0.118459	-0.228261	-0.562099
8	0.203763	-0.978027	-2.488742	8	0.385317	-1.357436	-2.367213
8	0.552884	-0.160903	-3.379935	8	0.642234	-0.524112	-3.283923
6	-0.454072	1.862667	-0.490757	6	-0.472713	1.822475	-0.582944
7	-1.655325	2.356536	-0.923499	7	-1.672389	2.256378	-1.079841
6	-1.612853	3.719797	-1.149154	6	-1.636571	3.584703	-1.458048
1	-2.466951	4.269529	-1.505466	1	-2.491300	4.083113	-1.882005
6	-0.365537	4.120400	-0.835501	6	-0.394493	4.027655	-1.180487
1	0.101337	5.090764	-0.860654	1	0.065450	4.993322	-1.307811
7	0.318044	2.990385	-0.421310	7	0.291026	2.956535	-0.636502
6	-2.862767	1.600603	-1.077775	6	-2.871158	1.477545	-1.179223
6	-3.204520	1.113726	-2.344121	6	-3.174177	0.849476	-2.392167
6	-4.429800	0.459086	-2.470637	6	-4.395036	0.179991	-2.479471
1	-4.724015	0.067906	-3.437916	1	-4.663970	-0.314534	-3.405984
6	-5.266797	0.292095	-1.380003	6	-5.261978	0.131660	-1.400727
1	-6.211289	-0.229419	-1.498443	1	-6.202707	-0.402776	-1.487032
6	-4.902123	0.784817	-0.136251	6	-4.932031	0.758172	-0.208576

1	-5.561407	0.638332	0.710632	1	-5.613450	0.699410	0.631383
6	-3.698129	1.460886	0.040469	6	-3.734281	1.454266	-0.073696
6	-2.310301	1.324014	-3.546818	6	-2.246085	0.928510	-3.585462
1	-1.287846	1.453090	-3.182294	1	-1.233987	1.101383	-3.209208
6	-2.299938	0.128904	-4.495347	6	-2.204832	-0.365453	-4.392382
1	-2.063125	-0.794250	-3.966192	1	-1.973797	-1.220084	-3.756735
1	-1.531537	0.275048	-5.257881	1	-1.417855	-0.299591	-5.146711
1	-3.259997	0.008090	-5.008193	1	-3.151157	-0.553262	-4.910658
6	-2.719795	2.589948	-4.305289	6	-2.636148	2.098849	-4.492728
1	-2.667410	3.481076	-3.675926	1	-2.602918	3.055559	-3.967034
1	-3.745601	2.501051	-4.678368	1	-3.650932	1.963079	-4.881413
1	-2.058782	2.746078	-5.162947	1	-1.951943	2.161051	-5.344217
6	-3.327055	2.063785	1.380599	6	-3.393765	2.186391	1.209372
1	-2.238369	1.999027	1.470457	1	-2.308091	2.126182	1.334577
6	-3.935506	1.318754	2.561314	6	-4.038880	1.562283	2.440676
1	-3.731784	0.249562	2.507655	1	-3.849939	0.489813	2.489938
1	-5.020157	1.461154	2.612198	1	-5.122104	1.722222	2.452573
1	-3.519769	1.705838	3.496445	1	-3.637746	2.029027	3.345262
6	-3.732668	3.539364	1.456194	6	-3.788295	3.664941	1.131336
1	-3.257402	4.141668	0.681610	1	-3.279174	4.189232	0.322095
1	-3.447426	3.958603	2.426444	1	-3.534720	4.172271	2.067778
1	-4.817722	3.639767	1.349893	1	-4.867723	3.762474	0.976171
6	1.658203	3.095777	0.071179	6	1.620987	3.127288	-0.134751
6	1.844792	3.696690	1.327846	6	1.774746	3.839792	1.066479
6	3.153202	3.907367	1.752554	6	3.071385	4.100018	1.499434
1	3.336556	4.370801	2.714711	1	3.228577	4.648722	2.420596
6	4.229528	3.527481	0.961454	6	4.167958	3.662139	0.768442
1	5.242596	3.700643	1.310364	1	5.171621	3.873639	1.123327
6	4.014469	2.927235	-0.267090	6	3.985139	2.957995	-0.409195
1	4.860067	2.633360	-0.878886	1	4.846672	2.621970	-0.975417
6	2.721671	2.706532	-0.745120	6	2.705151	2.684732	-0.894916
6	0.663188	4.059903	2.206521	6	0.571178	4.274017	1.880606
1	-0.154472	4.379212	1.553267	1	-0.241384	4.496590	1.182576
6	0.174073	2.825779	2.964920	6	0.092868	3.126802	2.771177
1	-0.020097	1.995118	2.283464	1	-0.074893	2.219359	2.188284
1	-0.747332	3.050146	3.512029	1	-0.841879	3.394858	3.274327
1	0.926825	2.497111	3.687516	1	0.838693	2.899993	3.538963
6	0.944206	5.210470	3.166344	6	0.811842	5.535410	2.702581
1	1.335982	6.087888	2.644263	1	1.199479	6.352541	2.087867
1	1.662780	4.926690	3.941357	1	1.517783	5.360518	3.520412
1	0.020968	5.501227	3.675304	1	-0.127193	5.865808	3.155372
6	2.501813	2.131531	-2.123644	6	2.523742	2.003133	-2.230360
1	1.462465	1.807597	-2.200423	1	1.485827	1.675339	-2.312658
6	3.353050	0.891947	-2.363462	6	3.380577	0.750019	-2.350688
1	3.087855	0.443426	-3.323245	1	3.142678	0.227474	-3.279747
1	3.168589	0.148701	-1.586000	1	3.175193	0.067390	-1.524483
1	4.424312	1.117547	-2.378145	1	4.451496	0.977128	-2.352632
6	2.743865	3.201734	-3.188685	6	2.798569	2.989326	-3.366667
1	2.541595	2.793840	-4.183328	1	2.625062	2.506787	-4.332931
1	3.781452	3.552410	-3.167800	1	3.835723	3.340917	-3.342397
1	2.093435	4.068733	-3.038581	1	2.146310	3.865455	-3.302102
6	0.496404	-1.854664	0.634725	6	0.487978	-1.793108	0.730190
7	1.699996	-2.476068	0.818328	7	1.691007	-2.388696	0.992882
6	1.598669	-3.587173	1.639090	6	1.574289	-3.436110	1.891935
1	2.454689	-4.190164	1.891416	1	2.427927	-4.008025	2.214590
6	0.301064	-3.691762	1.980169	6	0.268969	-3.527254	2.203873

1	-0.222768	-4.416257	2.580700	1	-0.267154	-4.209571	2.841852
7	-0.355702	-2.635701	1.365085	7	-0.377896	-2.526266	1.492768
6	2.940519	-2.120561	0.197702	6	2.953492	-2.053243	0.406707
6	3.874246	-1.402200	0.954937	6	3.823826	-1.237366	1.140660
6	5.109667	-1.133123	0.370709	6	5.076022	-0.970881	0.591998
1	5.852282	-0.571433	0.925024	1	5.769623	-0.333001	1.127171
6	5.403871	-1.585334	-0.906621	6	5.450045	-1.523898	-0.623258
1	6.372888	-1.370002	-1.345276	1	6.430829	-1.308601	-1.035061
6	4.466147	-2.306026	-1.628485	6	4.579476	-2.351003	-1.314809
1	4.706650	-2.646643	-2.628524	1	4.884862	-2.777167	-2.263089
6	3.210571	-2.590815	-1.093931	6	3.309590	-2.637196	-0.815877
6	3.527440	-0.917103	2.345899	6	3.402715	-0.661352	2.475149
1	2.874371	-1.668634	2.802803	1	2.725382	-1.383395	2.943879
6	4.742254	-0.760079	3.254159	6	4.569132	-0.447559	3.434533
1	5.353767	-1.666735	3.279779	1	5.177081	-1.350128	3.544938
1	4.414593	-0.541240	4.274310	1	4.188698	-0.168950	4.421302
1	5.378357	0.072243	2.936966	1	5.222373	0.365282	3.102317
6	2.741693	0.389211	2.262240	6	2.624222	0.635152	2.270895
1	1.850496	0.281875	1.636283	1	1.762779	0.485238	1.613572
1	3.358851	1.175396	1.822679	1	3.261300	1.394544	1.813136
1	2.431813	0.712426	3.260354	1	2.268294	1.019634	3.230982
6	2.204412	-3.420337	-1.863137	6	2.383867	-3.590300	-1.541413
1	1.209468	-3.096897	-1.547477	1	1.359687	-3.299365	-1.297518
6	2.366785	-4.904221	-1.521240	6	2.610035	-5.024773	-1.054274
1	2.229133	-5.094207	-0.454494	1	2.436607	-5.123580	0.019602
1	3.364716	-5.255864	-1.803337	1	3.636098	-5.345022	-1.263581
1	1.629351	-5.502215	-2.065057	1	1.928766	-5.710862	-1.566802
6	2.282216	-3.215546	-3.372513	6	2.520768	-3.522000	-3.058929
1	2.216079	-2.159864	-3.638984	1	2.422007	-2.498746	-3.423322
1	1.444611	-3.729817	-3.851842	1	1.728908	-4.116774	-3.522373
1	3.202644	-3.633433	-3.793970	1	3.476971	-3.932849	-3.399865
6	-1.774598	-2.490222	1.472778	6	-1.798785	-2.381015	1.570971
6	-2.574325	-2.769418	0.356771	6	-2.588972	-2.771781	0.481736
6	-3.955888	-2.720106	0.532917	6	-3.971895	-2.719391	0.647811
1	-4.605614	-2.907792	-0.312846	1	-4.616332	-2.994882	-0.177468
6	-4.510404	-2.451478	1.773268	6	-4.536309	-2.333573	1.852500
1	-5.589163	-2.438996	1.891769	1	-5.615902	-2.319502	1.963029
6	-3.694688	-2.192536	2.864345	6	-3.729706	-1.960741	2.916494
1	-4.144432	-1.978794	3.826523	1	-4.186400	-1.658389	3.851342
6	-2.307506	-2.184403	2.733879	6	-2.341978	-1.957480	2.792907
6	-1.964111	-3.170259	-0.969951	6	-1.967840	-3.268867	-0.807959
1	-1.088249	-2.534584	-1.125913	1	-1.146078	-2.587074	-1.047931
6	-1.498748	-4.628654	-0.932359	6	-1.389699	-4.677221	-0.641977
1	-0.759507	-4.805554	-0.147931	1	-0.618562	-4.722357	0.128930
1	-1.041217	-4.900383	-1.888529	1	-0.938261	-5.006348	-1.582830
1	-2.347165	-5.299290	-0.759164	1	-2.179354	-5.388621	-0.377468
6	-2.889794	-2.941475	-2.155750	6	-2.929654	-3.243000	-1.987557
1	-3.275626	-1.920230	-2.165660	1	-3.391792	-2.260736	-2.104700
1	-3.738195	-3.635011	-2.157167	1	-3.722716	-3.992137	-1.884131
1	-2.334777	-3.102953	-3.083418	1	-2.382501	-3.471905	-2.905606
6	-1.401702	-1.811478	3.893112	6	-1.444201	-1.469001	3.914152
1	-0.562746	-2.514731	3.904279	1	-0.591418	-2.151750	3.983590
6	-2.077468	-1.901713	5.255569	6	-2.117666	-1.454318	5.280723
1	-2.522726	-2.885875	5.427501	1	-2.547358	-2.427174	5.536235
1	-2.862794	-1.147214	5.367166	1	-2.914167	-0.705013	5.330333
1	-1.342107	-1.720231	6.043997	1	-1.384507	-1.195567	6.049470

Z	X	Y	Z		Z	X	Y	Z
6	-0.811659	-0.416023	3.677283		6	-0.883541	-0.086157	3.575678
1	-0.340483	-0.324140	2.696525		1	-0.424364	-0.067923	2.584723
1	-0.060913	-0.194630	4.442153		1	-0.130242	0.212982	4.310935
1	-1.595308	0.342672	3.742315		1	-1.681830	0.659941	3.587139

End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 137° (OST)

Z	X	Y	Z
46	0.123963	-0.257020	-0.627387
8	0.481750	-1.525922	-2.322649
8	0.652110	-0.652083	-3.231937
6	-0.458455	1.788194	-0.593607
7	-1.655372	2.204997	-1.114085
6	-1.604405	3.505269	-1.578759
1	-2.454650	3.985369	-2.031812
6	-0.357489	3.951163	-1.331203
1	0.112426	4.901915	-1.519813
7	0.317479	2.909918	-0.719930
6	-2.859488	1.430936	-1.185365
6	-3.167775	0.768621	-2.378844
6	-4.394061	0.106312	-2.446253
1	-4.667480	-0.412924	-3.357901
6	-5.261443	0.098561	-1.367525
1	-6.206504	-0.430634	-1.437279
6	-4.927342	0.760426	-0.195553
1	-5.611111	0.733772	0.643913
6	-3.725059	1.451733	-0.080738
6	-2.244370	0.805405	-3.578318
1	-1.232071	1.006602	-3.216495
6	-2.189699	-0.522815	-4.327004
1	-1.934241	-1.343706	-3.657660
1	-1.413542	-0.477258	-5.093903
1	-3.138904	-0.751165	-4.823332
6	-2.654240	1.927956	-4.535876
1	-2.636701	2.907440	-4.053283
1	-3.667095	1.758754	-4.916346
1	-1.972213	1.963535	-5.390608
6	-3.382072	2.226417	1.177089
1	-2.304296	2.118102	1.335776
6	-4.092681	1.699586	2.417902
1	-3.959481	0.623343	2.530262
1	-5.166284	1.913449	2.387108
1	-3.694603	2.193906	3.309072
6	-3.697913	3.718042	1.021518
1	-3.135958	4.181373	0.210403
1	-3.450731	4.252269	1.944551
1	-4.765407	3.861080	0.824709
6	1.647977	3.104394	-0.227781
6	1.802540	3.879379	0.933870
6	3.099508	4.152941	1.357801
1	3.256898	4.748275	2.249558
6	4.195643	3.670666	0.654848
1	5.199467	3.892117	1.003142
6	4.012229	2.912691	-0.488880
1	4.873460	2.545355	-1.035596
6	2.732105	2.624234	-0.965321
6	0.599974	4.370910	1.716284
1	-0.209350	4.552990	1.002812

End-on [Pd(IPr)$_2$(^{1}-O$_2$)] scan C-Pd-C = 132° (OST)

Z	X	Y	Z
46	0.133518	-0.280175	-0.699609
8	0.558377	-1.640993	-2.296521
8	0.686459	-0.788236	-3.240422
6	-0.478699	1.746204	-0.608321
7	-1.687395	2.144212	-1.117318
6	-1.655922	3.437680	-1.603122
1	-2.515891	3.900114	-2.055983
6	-0.411698	3.900517	-1.377556
1	0.045880	4.852774	-1.587675
7	0.283022	2.876359	-0.758587
6	-2.882012	1.354674	-1.178526
6	-3.172669	0.661030	-2.358946
6	-4.391036	-0.016056	-2.420980
1	-4.650833	-0.559681	-3.322315
6	-5.268957	-0.005600	-1.350802
1	-6.207855	-0.546204	-1.416205
6	-4.953802	0.689898	-0.193337
1	-5.646484	0.678412	0.639111
6	-3.759583	1.396186	-0.084032
6	-2.242119	0.684556	-3.553490
1	-1.232666	0.897388	-3.190015
6	-2.173794	-0.653731	-4.282200
1	-1.912145	-1.462126	-3.600281
1	-1.395478	-0.612835	-5.047005
1	-3.119372	-0.898166	-4.777839
6	-2.653232	1.790533	-4.529701
1	-2.645241	2.776856	-4.061087
1	-3.662323	1.608801	-4.914424
1	-1.965442	1.818310	-5.380053
6	-3.440725	2.209433	1.156064
1	-2.363631	2.119079	1.329882
6	-4.161230	1.709027	2.402393
1	-4.022070	0.637109	2.544047
1	-5.235810	1.914332	2.353712
1	-3.777142	2.229111	3.284975
6	-3.772431	3.692659	0.958491
1	-3.197929	4.145136	0.150353
1	-3.552837	4.250717	1.874352
1	-4.836993	3.816784	0.735009
6	1.619982	3.095041	-0.293370
6	1.788532	3.920914	0.830344
6	3.091420	4.213008	1.224642
1	3.260311	4.847453	2.086727
6	4.178068	3.697391	0.531731
1	5.186236	3.931578	0.858545
6	3.980890	2.889290	-0.575641
1	4.835371	2.494958	-1.113226
6	2.695547	2.583587	-1.024847
6	0.596192	4.447849	1.606255
1	-0.211205	4.631917	0.891061

6	0.112914	3.287174	2.677967	6	0.089299	3.391838	2.588269
1	-0.064359	2.347095	2.153124	1	-0.102847	2.444315	2.082673
1	-0.818138	3.595147	3.164694	1	-0.837240	3.725394	3.066552
1	0.859034	3.101850	3.456632	1	0.831015	3.210138	3.371750
6	0.847368	5.681801	2.454809	6	0.867490	5.766671	2.321535
1	1.240802	6.454498	1.788503	1	1.273772	6.520992	1.642000
1	1.551388	5.556599	3.283248	1	1.569791	5.643033	3.151723
1	-0.090239	6.046610	2.883528	1	-0.063216	6.155076	2.744437
6	2.549744	1.890954	-2.273139	6	2.484115	1.802895	-2.300072
1	1.514111	1.551524	-2.337563	1	1.495357	1.339789	-2.256241
6	3.418357	0.643344	-2.357704	6	3.480764	0.666274	-2.472398
1	3.172366	0.083578	-3.262665	1	3.181500	0.048652	-3.321996
1	3.233343	-0.009280	-1.503309	1	3.497211	0.028691	-1.587658
1	4.486614	0.881441	-2.384754	1	4.498063	1.027178	-2.658901
6	2.805242	2.839271	-3.445945	6	2.499078	2.749284	-3.502171
1	2.630165	2.320700	-4.393061	1	2.302690	2.189239	-4.420993
1	3.838476	3.202974	-3.441736	1	3.472522	3.241959	-3.601298
1	2.143306	3.709683	-3.407769	1	1.735160	3.526838	-3.410416
6	0.464479	-1.755460	0.771619	6	0.483005	-1.701137	0.803749
7	1.657547	-2.355604	1.067615	7	1.679924	-2.281325	1.124015
6	1.516602	-3.378750	1.990725	6	1.541504	-3.283188	2.070413
1	2.360108	-3.947860	2.343316	1	2.387925	-3.834021	2.444326
6	0.205807	-3.450490	2.283627	6	0.229221	-3.361803	2.353902
1	-0.347573	-4.110314	2.930542	1	-0.323323	-4.011655	3.011552
7	-0.419430	-2.462581	1.536187	7	-0.399439	-2.399212	1.576940
6	2.937716	-2.039044	0.509047	6	2.966536	-1.964856	0.578084
6	3.778929	-1.187893	1.236818	6	3.785375	-1.085940	1.298696
6	5.046035	-0.932728	0.717824	6	5.059469	-0.830423	0.797229
1	5.716457	-0.265990	1.247487	1	5.712259	-0.142106	1.321207
6	5.464624	-1.535227	-0.458664	6	5.508303	-1.461710	-0.352762
1	6.456489	-1.328724	-0.847803	1	6.504821	-1.254077	-0.729029
6	4.625369	-2.403442	-1.138497	6	4.693873	-2.362473	-1.020207
1	4.967359	-2.872007	-2.053769	1	5.060745	-2.857047	-1.911827
6	3.341436	-2.678685	-0.670182	6	3.403884	-2.639418	-0.569323
6	3.315766	-0.567579	2.536684	6	3.294977	-0.444051	2.577856
1	2.606358	-1.263863	2.996394	1	2.591522	-1.142169	3.044026
6	4.447793	-0.350189	3.535874	6	4.409586	-0.185658	3.586643
1	5.031880	-1.261142	3.694971	1	5.006797	-1.082728	3.773494
1	4.034315	-0.036124	4.498476	1	3.977642	0.141863	4.536573
1	5.130355	0.439835	3.207937	1	5.083082	0.608844	3.250855
6	2.572923	0.737242	2.267289	6	2.534618	0.841567	2.271021
1	1.737406	0.587068	1.577778	1	1.708509	0.662459	1.578006
1	3.245386	1.472022	1.820221	1	3.200633	1.575725	1.813637
1	2.184268	1.152651	3.201319	1	2.130597	1.272205	3.191447
6	2.453208	-3.678630	-1.379133	6	2.550433	-3.682817	-1.257890
1	1.417568	-3.401937	-1.171038	1	1.505421	-3.424980	-1.075721
6	2.697866	-5.088475	-0.832611	6	2.820263	-5.067780	-0.661540
1	2.503882	-5.150625	0.240452	1	2.609934	-5.101276	0.409749
1	3.734217	-5.395431	-1.008182	1	3.866392	-5.354827	-0.810530
1	2.041333	-5.807191	-1.332622	1	2.189633	-5.817655	-1.148972
6	2.626668	-3.665261	-2.894489	6	2.749153	-3.716490	-2.769942
1	2.519628	-2.657924	-3.298243	1	2.629499	-2.725797	-3.209319
1	1.856556	-4.290309	-3.354572	1	1.998453	-4.370880	-3.221103
1	3.597978	-4.071897	-3.195544	1	3.732881	-4.114480	-3.041059
6	-1.840033	-2.304179	1.592892	6	-1.823256	-2.262419	1.619323
6	-2.623518	-2.742544	0.517180	6	-2.592789	-2.750778	0.554977

6	-4.007326	-2.680282	0.672428		6	-3.978250	-2.714057	0.704380
1	-4.647739	-2.990912	-0.143370		1	-4.608959	-3.062412	-0.103604
6	-4.578378	-2.240327	1.855266		6	-4.563173	-2.254202	1.872612
1	-5.658641	-2.220939	1.958363		1	-5.643922	-2.257064	1.972213
6	-3.778048	-1.820543	2.906317		6	-3.776209	-1.787672	2.913890
1	-4.239519	-1.478906	3.825243		1	-4.248214	-1.433938	3.822819
6	-2.389743	-1.824271	2.790504		6	-2.387950	-1.761889	2.801581
6	-1.994654	-3.296150	-0.745774		6	-1.949174	-3.332167	-0.688169
1	-1.174834	-2.621816	-1.014316		1	-1.145196	-2.648805	-0.981431
6	-1.408802	-4.692678	-0.515987		6	-1.329340	-4.705873	-0.412621
1	-0.637274	-4.700654	0.255603		1	-0.555160	-4.671208	0.355598
1	-0.955620	-5.060784	-1.441408		1	-0.870334	-5.093468	-1.327105
1	-2.194970	-5.395597	-0.220159		1	-2.098054	-5.416854	-0.091084
6	-2.953975	-3.333520	-1.927360		6	-2.907468	-3.436002	-1.866707
1	-3.424203	-2.362251	-2.093146		1	-3.405000	-2.484664	-2.064766
1	-3.741441	-4.082908	-1.788567		1	-3.673793	-4.201703	-1.701210
1	-2.403736	-3.602652	-2.832524		1	-2.350323	-3.720391	-2.762859
6	-1.495463	-1.289723	3.892757		6	-1.509236	-1.180749	3.892704
1	-0.641535	-1.967630	3.989563		1	-0.643943	-1.840412	4.011595
6	-2.171254	-1.222498	5.256618		6	-2.192523	-1.088839	5.251412
1	-2.600083	-2.185284	5.549081		1	-2.604862	-2.051147	5.568167
1	-2.968797	-0.472906	5.275582		1	-3.003769	-0.353835	5.247030
1	-1.439903	-0.932791	6.016020		1	-1.469936	-0.765402	6.005575
6	-0.937420	0.080094	3.500210		6	-0.972931	0.187523	3.465842
1	-0.487192	0.064678	2.504733		1	-0.519854	0.153319	2.472388
1	-0.178129	0.404606	4.218293		1	-0.220637	0.542560	4.176712
1	-1.735905	0.825977	3.494204		1	-1.783193	0.920041	3.439420

End-on [Pd(IPr)₂(^{1}-O₂)] scan C-Pd-C = 127° (OST) — **Side-on [Pd(IPr)₂]-O₂ scan Pd-O = 2.0 Å (OST)**

46	0.145568	-0.324864	-0.764301		46	-0.124521	0.271298	-0.676635
8	0.545260	-1.783938	-2.265262		8	-0.167116	-0.197315	-2.620470
8	0.731694	-0.990282	-3.255897		8	-0.310067	1.077993	-2.497273
6	-0.463538	1.699353	-0.646239		7	-0.469321	-2.941911	-0.518426
7	-1.680527	2.095087	-1.138249		7	1.532389	-2.366742	-0.957470
6	-1.657973	3.388201	-1.626068		7	0.483701	2.640143	1.318192
1	-2.521585	3.844719	-2.077505		7	-1.579499	2.560366	0.790519
6	-0.412175	3.853493	-1.419366		6	0.389129	-1.888278	-0.375547
1	0.041842	4.803866	-1.644960		6	0.108284	-4.012252	-1.182216
7	0.294166	2.832091	-0.808134		1	-0.433883	-4.921899	-1.379353
6	-2.873793	1.302499	-1.195218		6	1.374752	-3.647324	-1.459424
6	-3.135193	0.554928	-2.350488		1	2.176267	-4.174976	-1.947653
6	-4.348368	-0.131041	-2.407940		6	-1.792277	-3.048050	0.017810
1	-4.583827	-0.718891	-3.287741		6	-1.944107	-3.649467	1.276324
6	-5.253795	-0.072386	-1.361849		6	-3.238740	-3.823611	1.757452
1	-6.188021	-0.621365	-1.423948		1	-3.391670	-4.279987	2.728963
6	-4.973591	0.685681	-0.236042		6	-4.336971	-3.421290	1.009442
1	-5.689979	0.718421	0.575772		6	-4.158091	-2.845046	-0.237180
6	-3.784112	1.401419	-0.132120		1	-5.021013	-2.542833	-0.821219
6	-2.182631	0.538734	-3.527904		6	-2.880487	-2.658250	-0.766211
1	-1.173046	0.724354	-3.148887		6	-0.742049	-4.069831	2.095589
6	-2.141782	-0.803802	-4.249666		1	0.090442	-4.226170	1.403709
1	-1.921203	-1.618275	-3.560307		6	-2.705220	-2.104279	-2.159708
1	-1.345118	-0.790672	-4.996046		1	-1.638763	-1.955699	-2.331057
6	-3.083241	-1.018429	-4.766656		6	2.789839	-1.683984	-1.005961
6	-2.540534	1.650794	-4.518689		6	3.282429	-1.252094	-2.242424
1	-2.504133	2.640253	-4.058502		6	4.544712	-0.655112	-2.262835
					1	4.953361	-0.313404	-3.207936

1	-3.549195	1.500176	-4.917831	6	5.274088	-0.487335	-1.100696
1	-1.838599	1.646497	-5.357802	6	4.766334	-0.934038	0.111220
6	-3.517193	2.295098	1.063783	1	5.349551	-0.796340	1.012742
1	-2.436829	2.289087	1.238955	6	3.526302	-1.558597	0.185536
6	-4.204472	1.812725	2.336414	6	2.532979	-1.450218	-3.543465
1	-4.011394	0.756029	2.520239	1	1.513982	-1.760617	-3.306216
1	-5.288350	1.959704	2.286609	6	3.012556	-2.135579	1.490670
1	-3.843809	2.388476	3.194020	1	1.960001	-1.844663	1.572364
6	-3.951474	3.738765	0.787879	6	-0.411201	1.865654	0.632465
1	-3.416418	4.182259	-0.051711	6	-0.111722	3.759133	1.882518
1	-3.764280	4.362472	1.667845	1	0.453532	4.480512	2.448510
1	-5.023398	3.775639	0.568751	6	-1.415089	3.705075	1.553276
6	1.642136	3.052313	-0.374163	1	-2.238043	4.360795	1.782283
6	1.842039	3.926464	0.707689	6	1.888387	2.413410	1.459402
6	3.156147	4.209372	1.071853	6	2.731992	2.666159	0.370689
1	3.349470	4.879891	1.900606	6	4.103732	2.542701	0.584053
6	4.222768	3.635452	0.394823	1	4.786591	2.709046	-0.239859
1	5.239526	3.859580	0.701442	6	4.607626	2.222011	1.833831
6	3.995284	2.783157	-0.673261	6	3.749097	1.986519	2.897290
1	4.834630	2.344776	-1.199854	1	4.158661	1.737103	3.869091
6	2.699136	2.490058	-1.097961	6	2.368126	2.060449	2.729017
6	0.672362	4.520246	1.471649	6	2.178487	3.107492	-0.968341
1	-0.118657	4.740718	0.748841	1	1.262749	2.534096	-1.140546
6	0.098327	3.504599	2.459195	6	1.405443	1.734500	3.854708
1	-0.137634	2.561190	1.964904	1	0.599034	2.474707	3.826989
1	-0.815637	3.893127	2.919880	6	-2.843609	2.236720	0.203215
1	0.818451	3.296172	3.255576	6	-3.145739	2.740856	-1.068363
6	1.004951	5.829033	2.179039	6	-4.419014	2.481870	-1.573345
1	1.454927	6.556946	1.498219	1	-4.685566	2.850304	-2.556992
1	1.692394	5.675567	3.016793	6	-5.343879	1.755267	-0.840700
1	0.091509	6.267461	2.590397	6	-5.019862	1.274254	0.418733
6	2.453172	1.670136	-2.342244	1	-5.754432	0.712393	0.983705
1	1.505671	1.138061	-2.215595	6	-3.765630	1.517513	0.973318
6	3.511236	0.605600	-2.585981	6	-2.156226	3.581467	-1.848070
1	3.178086	-0.051465	-3.392086	1	-1.153429	3.288664	-1.526348
1	3.659626	-0.008997	-1.697218	6	-3.391751	1.010565	2.348631
1	4.475771	1.035697	-2.878162	1	-2.684172	1.727119	2.779921
6	2.302478	2.588219	-3.557261	6	2.032230	1.805829	5.241412
1	2.083020	1.991820	-4.447480	1	2.514354	2.770642	5.423603
1	3.225120	3.150585	-3.737820	1	1.260220	1.663747	6.002504
1	1.487975	3.305716	-3.424576	1	2.778024	1.018005	5.388606
6	0.475999	-1.640711	0.856571	6	0.764960	0.364299	3.621312
7	1.670950	-2.200689	1.218318	1	1.507390	-0.427137	3.747771
6	1.524026	-3.156284	2.210025	1	-0.041095	0.189612	4.340609
1	2.367048	-3.687235	2.618843	1	0.352851	0.278974	2.613407
6	0.208820	-3.225451	2.481598	6	1.812632	4.594359	-0.948551
1	-0.349643	-3.845267	3.162806	1	1.065005	4.824541	-0.186309
7	-0.413472	-2.303546	1.651728	1	2.698769	5.208125	-0.754759
6	2.963598	-1.912060	0.668912	1	1.400483	4.890692	-1.918226
6	3.784007	-1.013513	1.363248	6	3.112905	2.808066	-2.132267
6	5.060810	-0.779271	0.858736	1	2.594507	3.001786	-3.074872
1	5.714072	-0.076665	1.362475	1	4.006489	3.441965	-2.115027
6	5.511826	-1.450870	-0.267378	1	3.428829	1.763051	-2.128575
1	6.510125	-1.258945	-0.647346	6	-4.580812	0.914075	3.299189
6	4.698251	-2.374445	-0.903868	1	-5.147780	1.848595	3.341434
1	5.067964	-2.903266	-1.774350	1	-5.265250	0.111710	3.006790

6	3.405741	-2.632523	-0.448402	1	-4.229147	0.682353	4.308430
6	3.292195	-0.333519	2.621989	6	-2.680337	-0.335501	2.234832
1	2.614409	-1.031721	3.125056	1	-2.372068	-0.687828	3.223343
6	4.409823	-0.002382	3.605430	1	-3.349266	-1.081213	1.800215
1	5.034247	-0.873602	3.823308	1	-1.795292	-0.268638	1.596121
1	3.979113	0.352830	4.545872	6	-2.347313	5.067232	-1.530282
1	5.056652	0.795801	3.228255	1	-1.617585	5.669167	-2.080495
6	2.492537	0.916689	2.274549	1	-3.349767	5.397331	-1.821921
1	1.670751	0.689890	1.591287	1	-2.218379	5.276543	-0.466273
1	3.135883	1.653615	1.790644	6	-2.234311	3.351540	-3.354367
1	2.078919	1.366254	3.181497	1	-2.144617	2.291893	-3.595502
6	2.559875	-3.708585	-1.094485	1	-3.165709	3.741540	-3.777858
1	1.512921	-3.442644	-0.938565	1	-1.410053	3.874850	-3.847043
6	2.823857	-5.061292	-0.425274	6	-3.214989	-3.098654	-3.203542
1	2.598880	-5.041485	0.643413	1	-2.704744	-4.062919	-3.120665
1	3.872365	-5.352981	-0.545641	1	-4.289312	-3.278126	-3.090826
1	2.200976	-5.835945	-0.882978	1	-3.042433	-2.708678	-4.210991
6	2.776623	-3.819964	-2.600256	6	-3.372404	-0.742277	-2.308347
1	2.660726	-2.854211	-3.092904	1	-3.142749	-0.315531	-3.288363
1	2.031495	-4.497718	-3.025194	1	-4.460734	-0.808425	-2.214468
1	3.763796	-4.230269	-2.838977	1	-3.008050	-0.049327	-1.547616
6	-1.839433	-2.177355	1.670027	6	-0.955414	-5.380501	2.846586
6	-2.591800	-2.728263	0.623859	1	-1.286831	-6.178380	2.176386
6	-3.979205	-2.700208	0.756929	1	-0.018930	-5.696030	3.315531
1	-4.596780	-3.096356	-0.039058	1	-1.697131	-5.278947	3.644660
6	-4.582370	-2.191104	1.894828	6	-0.334542	-2.946221	3.047417
1	-5.664031	-2.201783	1.983026	1	0.580814	-3.209764	3.586955
6	-3.812124	-1.666849	2.920858	1	-0.159539	-2.020452	2.497241
1	-4.297719	-1.277524	3.807759	1	-1.121391	-2.759034	3.785338
6	-2.423161	-1.629898	2.821977	6	3.095630	-3.666180	1.485596
6	-1.930527	-3.369586	-0.579894	1	2.517552	-4.115864	0.677652
1	-1.126628	-2.699904	-0.901583	1	4.136955	-3.987563	1.379055
6	-1.308303	-4.724162	-0.225878	1	2.715674	-4.066589	2.430879
1	-0.542019	-4.646741	0.547187	6	3.744000	-1.607685	2.717208
1	-0.838347	-5.156808	-1.114177	1	3.748792	-0.517459	2.746899
1	-2.077841	-5.420575	0.124409	1	3.252176	-1.974157	3.623096
6	-2.874448	-3.540968	-1.762317	1	4.780343	-1.961069	2.750562
1	-3.380849	-2.606131	-2.010312	6	2.423609	-0.159748	-4.352193
1	-3.633658	-4.307135	-1.568933	1	3.404808	0.199202	-4.679418
1	-2.303464	-3.860029	-2.637766	1	1.819785	-0.335730	-5.246840
6	-1.563212	-0.993360	3.897182	1	1.938038	0.625049	-3.772958
1	-0.698875	-1.644521	4.061402	6	3.195447	-2.549259	-4.378392
6	-2.267377	-0.837760	5.239313	1	2.628502	-2.723613	-5.297754
1	-2.678925	-1.785499	5.598232	1	4.214416	-2.264402	-4.659689
1	-3.082645	-0.109079	5.185923	1	3.259074	-3.496075	-3.835035
1	-1.557849	-0.472147	5.986584	1	-5.338775	-3.563799	1.402012
6	-1.020923	0.353721	3.414443	1	6.247826	-0.009140	-1.134930
1	-0.563210	0.274716	2.426145	1	-6.327847	1.561298	-1.255638
1	-0.270670	0.736244	4.112855	1	5.680616	2.150833	1.981375
1	-1.827518	1.087774	3.352612				

Side-on [Pd(IPr)₂]-O₂ scan Pd-O = 2.2 Å (OST)				Side-on [Pd(IPr)₂]-O₂ scan Pd-O = 2.3 Å (OST)			
46	0.034643	-0.088435	-0.544724	46	0.034231	-0.047892	-0.574218
8	-0.145441	0.404768	-2.681128	8	-0.159644	0.547342	-2.787386
8	0.174843	-0.827702	-2.612025	8	0.140834	-0.681749	-2.782580
7	0.238787	3.022753	-0.007899	7	0.202158	3.035669	0.051378
7	-1.745209	2.437544	-0.514861	7	-1.781895	2.448154	-0.455750

7	-0.240031	-2.916842	0.785349	7	-0.203681	-2.969450	0.507505
7	1.762440	-2.568403	0.154359	7	1.794634	-2.556951	-0.099202
6	-0.542156	1.907053	-0.127309	6	-0.564389	1.916733	-0.118815
6	-0.439894	4.184513	-0.337975	6	-0.499833	4.203068	-0.199859
1	0.035063	5.150622	-0.304841	1	-0.039180	5.173167	-0.117798
6	-1.694191	3.813843	-0.655008	6	-1.753873	3.830892	-0.517098
1	-2.554356	4.391070	-0.946922	1	-2.627643	4.410124	-0.760703
6	1.593434	3.082079	0.442289	6	1.558888	3.088588	0.496657
6	1.825372	3.464415	1.772664	6	1.793440	3.405650	1.843720
6	3.147970	3.627638	2.173291	6	3.116227	3.564389	2.245715
1	3.366707	3.922972	3.193149	1	3.336671	3.809577	3.278395
6	4.192808	3.404752	1.286158	6	4.158860	3.398117	1.343741
6	3.933668	3.026207	-0.019925	6	3.897166	3.079655	0.022153
1	4.756133	2.861167	-0.707718	1	4.717887	2.955422	-0.676301
6	2.623396	2.878270	-0.477155	6	2.586374	2.938364	-0.435755
6	0.675361	3.641832	2.742417	6	0.647831	3.511254	2.829357
1	-0.200523	3.951364	2.164224	1	-0.239178	3.831766	2.274714
6	2.345917	2.583820	-1.932833	6	2.304697	2.701189	-1.900935
1	1.275067	2.405602	-2.044731	1	1.236177	2.509890	-2.014002
6	-2.964036	1.711949	-0.699677	6	-2.991757	1.712979	-0.661158
6	-3.488208	1.581867	-1.991134	6	-3.529301	1.636607	-1.951216
6	-4.722645	0.944549	-2.125067	6	-4.752984	0.982630	-2.102748
1	-5.153759	0.828758	-3.113452	1	-5.193546	0.905659	-3.090727
6	-5.387978	0.440059	-1.023048	6	-5.396428	0.414165	-1.018901
6	-4.847261	0.586071	0.247176	6	-4.844306	0.510654	0.251031
1	-5.379741	0.185812	1.100760	1	-5.360386	0.061129	1.090091
6	-3.638115	1.245669	0.442100	6	-3.644582	1.181582	0.464448
6	-2.790004	2.132232	-3.217985	6	-2.857456	2.263528	-3.155731
1	-1.763553	2.380842	-2.937999	1	-1.830957	2.512716	-2.876336
6	-3.093350	1.506545	1.833590	6	-3.089443	1.387318	1.860772
1	-2.023153	1.275295	1.803099	1	-2.014523	1.183812	1.807785
6	0.560829	-1.925947	0.289728	6	0.585427	-1.939710	0.078027
6	0.436508	-4.115218	0.947526	6	0.487032	-4.167374	0.592526
1	-0.053025	-4.998793	1.321361	1	0.009102	-5.079103	0.909435
6	1.705589	-3.890546	0.558744	6	1.753314	-3.903009	0.219048
1	2.570486	-4.531157	0.537513	1	2.625033	-4.531440	0.156013
6	-1.630620	-2.825254	1.098406	6	-1.592864	-2.906227	0.833448
6	-2.562289	-2.915140	0.063127	6	-2.530377	-2.944464	-0.200100
6	-3.912310	-2.956020	0.414444	6	-3.877687	-3.008557	0.156740
1	-4.662189	-3.013569	-0.366756	1	-4.632673	-3.026479	-0.621289
6	-4.301528	-2.949213	1.742198	6	-4.258700	-3.069278	1.485999
6	-3.351500	-2.866386	2.753184	6	-3.303080	-3.035693	2.494178
1	-3.674528	-2.853723	3.787615	1	-3.619382	-3.076868	3.530039
6	-1.995471	-2.783027	2.452620	6	-1.948741	-2.935417	2.189772
6	-2.135662	-3.048582	-1.380619	6	-2.106761	-2.998826	-1.650016
1	-1.084898	-2.760960	-1.449059	1	-1.070942	-2.659699	-1.708430
6	-0.940500	-2.606788	3.526117	6	-0.886863	-2.812741	3.263889
1	-0.077070	-3.219901	3.245570	1	-0.016143	-3.389969	2.934433
6	2.990243	-1.976680	-0.273559	6	3.013922	-1.921811	-0.486901
6	3.426549	-2.183211	-1.588887	6	3.460387	-2.051972	-1.808344
6	4.676592	-1.674514	-1.935504	6	4.705600	-1.509802	-2.119941
1	5.046166	-1.815896	-2.944935	1	5.083283	-1.593392	-3.132939
6	5.444163	-0.973823	-1.017419	6	5.457790	-0.848007	-1.161479
6	4.983205	-0.778374	0.274679	6	4.985145	-0.724181	0.135501
1	5.590204	-0.231114	0.988225	1	5.580393	-0.205055	0.879252
6	3.753707	-1.294633	0.678547	6	3.760344	-1.276594	0.503944

6	2.600889	-2.959594	-2.592564	6	2.648826	-2.781652	-2.857687
1	1.568777	-2.965937	-2.232664	1	1.618731	-2.835699	-2.495809
6	3.302147	-1.172875	2.115734	6	3.297196	-1.234883	1.942302
1	2.273710	-1.534409	2.176280	1	2.261780	-1.579707	1.969877
6	-1.389320	-3.062949	4.908597	6	-1.314295	-3.369646	4.615953
1	-1.757083	-4.093069	4.898974	1	-1.668002	-4.401826	4.538710
1	-0.549675	-3.008945	5.606828	1	-0.467895	-3.351709	5.307973
1	-2.181675	-2.421558	5.307428	1	-2.110763	-2.768727	5.066282
6	-0.469280	-1.150036	3.559701	6	-0.440659	-1.353169	3.391929
1	-1.272608	-0.499709	3.916737	1	-1.249101	-0.744945	3.806748
1	0.382747	-1.037910	4.238041	1	0.420537	-1.272575	4.063200
1	-0.172334	-0.800320	2.566941	1	-0.167480	-0.929176	2.421071
6	-2.260858	-4.504077	-1.834464	6	-2.164591	-4.439475	-2.161948
1	-1.661448	-5.169869	-1.206610	1	-1.531744	-5.101057	-1.563331
1	-3.301221	-4.842485	-1.785870	1	-3.187614	-4.828635	-2.125503
1	-1.916969	-4.610951	-2.867759	1	-1.819629	-4.487974	-3.199294
6	-2.902124	-2.103220	-2.295338	6	-2.919130	-2.056816	-2.527472
1	-2.494950	-2.156922	-3.308474	1	-2.511786	-2.053752	-3.541999
1	-3.967471	-2.349543	-2.348655	1	-3.971673	-2.351343	-2.591756
1	-2.808427	-1.074116	-1.945776	1	-2.874089	-1.038240	-2.140042
6	4.163526	-2.052101	3.023158	6	4.134227	-2.185237	2.799655
1	4.135806	-3.098801	2.706815	1	4.085868	-3.210625	2.422165
1	5.208720	-1.726549	3.010022	1	5.186152	-1.881896	2.809757
1	3.807004	-1.998821	4.056600	1	3.773058	-2.185489	3.832892
6	3.289803	0.276237	2.577356	6	3.306065	0.181603	2.495809
1	2.895207	0.347213	3.595227	1	2.900685	0.192951	3.511744
1	4.292002	0.714172	2.578905	1	4.315476	0.600612	2.537772
1	2.659767	0.877603	1.920876	1	2.694045	0.835739	1.873962
6	3.090871	-4.407294	-2.685147	6	3.172018	-4.207938	-3.047211
1	2.477243	-4.973133	-3.392702	1	2.563627	-4.742947	-3.782665
1	4.128421	-4.441352	-3.033155	1	4.205579	-4.194058	-3.408362
1	3.045463	-4.916439	-1.719625	1	3.151703	-4.777807	-2.115346
6	2.593664	-2.313481	-3.975362	6	2.620259	-2.047121	-4.195731
1	2.264635	-1.275792	-3.920322	1	2.258052	-1.026289	-4.074852
1	3.581123	-2.351704	-4.446620	1	3.608489	-2.021475	-4.665795
1	1.898479	-2.849194	-4.627743	1	1.943491	-2.561837	-4.883504
6	2.716648	3.789071	-2.798589	6	2.651803	3.946595	-2.718213
1	2.178936	4.688038	-2.483140	1	2.100426	4.823049	-2.365095
1	3.788959	4.003403	-2.741040	1	3.720634	4.176257	-2.655178
1	2.467688	3.592952	-3.845720	1	2.402236	3.789154	-3.771740
6	3.053996	1.318500	-2.396491	6	3.029583	1.467160	-2.419611
1	2.779319	1.092350	-3.430323	1	2.752249	1.279556	-3.460385
1	4.142632	1.417249	-2.349552	1	4.116802	1.580863	-2.375195
1	2.763234	0.469544	-1.775408	1	2.756431	0.588866	-1.831872
6	0.927652	4.717769	3.792868	6	0.886680	4.536661	3.931955
1	1.213968	5.669192	3.335998	1	1.148131	5.516543	3.522775
1	0.020265	4.881252	4.381048	1	-0.018766	4.649391	4.534870
1	1.716639	4.426386	4.492982	1	1.687973	4.227323	4.610135
6	0.334045	2.302536	3.397497	6	0.339127	2.132647	3.415651
1	-0.557413	2.397941	4.025482	1	-0.550020	2.175999	4.052630
1	0.148146	1.534167	2.643870	1	0.165162	1.401622	2.622888
1	1.160190	1.962814	4.029264	1	1.176455	1.778059	4.024039
6	-3.264997	2.978201	2.226863	6	-3.293010	2.833436	2.327204
1	-2.745904	3.659481	1.552115	1	-2.801741	3.560130	1.679391
1	-4.326390	3.247401	2.232923	1	-4.360897	3.073576	2.360548
1	-2.870852	3.143786	3.234477	1	-2.888738	2.961078	3.336425

6	-3.729736	0.634014	2.904998	6	-3.690975	0.448744	2.896057
1	-3.660466	-0.424864	2.657249	1	-3.594104	-0.595313	2.599199
1	-3.219733	0.795410	3.859040	1	-3.176324	0.581557	3.852028
1	-4.784296	0.888507	3.058500	1	-4.750673	0.665524	3.070305
6	-2.711071	1.112732	-4.352753	6	-2.782059	1.310471	-4.347142
1	-3.703693	0.854752	-4.735526	1	-3.776841	1.069622	-4.735582
1	-2.136216	1.531253	-5.183797	1	-2.216905	1.778744	-5.158016
1	-2.210227	0.201993	-4.027212	1	-2.275067	0.384477	-4.079205
6	-3.487163	3.405640	-3.705305	6	-3.579926	3.551256	-3.561714
1	-2.954594	3.828879	-4.562304	1	-3.068642	4.027416	-4.403798
1	-4.512825	3.187494	-4.020159	1	-4.608164	3.335636	-3.869645
1	-3.539048	4.172306	-2.928148	1	-3.627458	4.273739	-2.743280
1	5.218058	3.530079	1.619809	1	5.184346	3.518598	1.678329
1	-6.337618	-0.069958	-1.149660	1	-6.337958	-0.107073	-1.159552
1	6.409537	-0.575842	-1.313513	1	6.419885	-0.423061	-1.429571
1	-5.354987	-3.004176	1.997847	1	-5.310566	-3.139344	1.744607

Side-on [Pd(IPr)$_2$]-O$_2$ scan Pd-O = 2.4 Å (OST)				Side-on [Pd(IPr)$_2$]-O$_2$ scan Pd-O = 2.6 Å (OST)			
46	0.025051	-0.043392	-0.387740	46	0.002623	-0.005600	-0.181373
8	-0.137722	0.503491	-2.718902	8	-0.026747	-0.513841	-2.731022
8	0.108815	-0.721784	-2.688319	8	-0.024932	0.704680	-2.682298
7	0.195762	3.051780	0.116978	7	-0.547780	-3.015082	0.298498
7	-1.780555	2.466279	-0.421925	7	1.485743	-2.703680	-0.255469
7	-0.194757	-2.987589	0.615587	7	0.552200	3.006814	0.349116
7	1.790775	-2.563115	-0.025183	7	-1.482312	2.704651	-0.205864
6	-0.568578	1.934074	-0.067865	6	0.340755	-2.009684	0.037025
6	-0.502789	4.220400	-0.137632	6	0.015270	-4.272416	0.153899
1	-0.043671	5.190158	-0.044082	1	-0.551758	-5.172700	0.320731
6	-1.752252	3.849690	-0.474382	6	1.301082	-4.075041	-0.192401
1	-2.623144	4.429728	-0.726316	1	2.103207	-4.768187	-0.378404
6	1.549971	3.098578	0.570131	6	-1.911904	-2.871740	0.697560
6	1.779281	3.407023	1.919948	6	-2.219332	-3.034543	2.056788
6	3.100671	3.561951	2.328012	6	-3.564089	-3.041386	2.414374
1	3.317306	3.801282	3.362845	1	-3.841730	-3.171952	3.454001
6	4.146821	3.397909	1.429619	6	-4.556982	-2.870071	1.457539
6	3.890242	3.084275	0.105835	6	-4.221800	-2.687612	0.126863
1	4.713833	2.959802	-0.589231	1	-5.004155	-2.549172	-0.611709
6	2.581076	2.947649	-0.357989	6	-2.888473	-2.700101	-0.284021
6	0.629041	3.503441	2.900972	6	-1.116803	-3.136374	3.090026
1	-0.252670	3.839631	2.346931	1	-0.267832	-3.642885	2.619613
6	2.304789	2.712757	-1.824721	6	-2.533178	-2.588597	-1.748372
1	1.235618	2.527249	-1.941733	1	-1.450925	-2.464554	-1.820065
6	-2.989061	1.735547	-0.648983	6	2.764572	-2.134776	-0.546819
6	-3.516289	1.682224	-1.944461	6	3.264650	-2.238507	-1.849917
6	-4.749856	1.051806	-2.114290	6	4.559196	-1.774897	-2.085969
1	-5.184542	0.995627	-3.106345	1	4.975340	-1.846505	-3.085081
6	-5.409423	0.476515	-1.043639	6	5.305120	-1.203905	-1.070880
6	-4.860934	0.537983	0.230120	6	4.777438	-1.094601	0.208627
1	-5.386617	0.079279	1.058378	1	5.367910	-0.631304	0.989299
6	-3.654031	1.190065	0.462232	6	3.506712	-1.576717	0.507422
6	-2.815317	2.296991	-3.138247	6	2.459052	-2.840730	-2.983000
1	-1.790540	2.532457	-2.840594	1	1.421571	-2.922688	-2.647692
6	-3.102574	1.363845	1.863442	6	2.953044	-1.536634	1.917849
1	-2.026710	1.166784	1.806011	1	1.915682	-1.192192	1.834170
6	0.583086	-1.950814	0.181885	6	-0.337554	2.006551	0.076564
6	0.500162	-4.184686	0.673058	6	-0.009550	4.266702	0.221669
1	0.030647	-5.101044	0.989157	1	0.558752	5.164169	0.398870

6	1.758377	-3.912871	0.278468	6	-1.296023	4.075024	-0.125359
1	2.630169	-4.538475	0.192736	1	-2.097784	4.771428	-0.300271
6	-1.574807	-2.933787	0.980030	6	1.917134	2.857730	0.744532
6	-2.540448	-2.961627	-0.027028	6	2.895054	2.724620	-0.241368
6	-3.876980	-3.046119	0.365321	6	4.228532	2.707120	0.169099
1	-4.652406	-3.061865	-0.392622	1	5.011488	2.596404	-0.573720
6	-4.220983	-3.133473	1.703122	6	4.562479	2.849689	1.504849
6	-3.238117	-3.103247	2.685191	6	3.568126	2.984044	2.466178
1	-3.525339	-3.158444	3.728802	1	3.844784	3.083765	3.509529
6	-1.893899	-2.985510	2.345457	6	2.223555	2.979392	2.108228
6	-2.160331	-2.981099	-1.489566	6	2.542134	2.648283	-1.708264
1	-1.118067	-2.666999	-1.568399	1	1.456585	2.564294	-1.786070
6	-0.807052	-2.859425	3.393561	6	1.120888	3.040487	3.144291
1	0.071592	-3.401034	3.026940	1	0.264177	3.545343	2.686547
6	3.005924	-1.918677	-0.410757	6	-2.765366	2.140571	-0.489581
6	3.457546	-2.046876	-1.730589	6	-3.291091	2.277670	-1.779724
6	4.701550	-1.499782	-2.038805	6	-4.588654	1.816011	-2.003514
1	5.082668	-1.582440	-3.050664	1	-5.023371	1.912521	-2.992557
6	5.448030	-0.834821	-1.078374	6	-5.314115	1.216320	-0.990434
6	4.970506	-0.712706	0.217096	6	-4.762641	1.077004	0.276039
1	5.561774	-0.191692	0.962597	1	-5.337766	0.593128	1.055603
6	3.747167	-1.270170	0.582440	6	-3.487959	1.555061	0.563909
6	2.652635	-2.778249	-2.783852	6	-2.512016	2.913741	-2.912753
1	1.623782	-2.846227	-2.420931	1	-1.469046	2.996352	-2.595863
6	3.283061	-1.235713	2.020842	6	-2.911239	1.483550	1.963810
1	2.242885	-1.565816	2.043733	1	-1.877776	1.133531	1.855713
6	-1.181228	-3.462880	4.741580	6	1.498406	3.827842	4.393584
1	-1.509039	-4.502101	4.646183	1	1.861658	4.829667	4.147105
1	-0.316507	-3.439744	5.410460	1	0.624944	3.931847	5.043262
1	-1.980581	-2.896791	5.230261	1	2.272934	3.318692	4.975544
6	-0.403616	-1.389862	3.544290	6	0.674895	1.619731	3.498294
1	-1.227339	-0.813267	3.974998	1	1.478120	1.086318	4.015603
1	0.460563	-1.294821	4.209894	1	-0.198260	1.642475	4.158096
1	-0.151097	-0.943056	2.577887	1	0.418647	1.054294	2.596843
6	-2.272831	-4.401486	-2.046352	6	2.974548	3.920808	-2.437039
1	-1.640827	-5.099220	-1.489206	1	2.514699	4.809536	-1.995064
1	-3.304451	-4.764838	-1.991450	1	4.060965	4.050515	-2.395833
1	-1.960692	-4.424300	-3.094924	1	2.681192	3.874061	-3.490231
6	-2.974586	-1.988304	-2.307710	6	3.129716	1.399482	-2.353299
1	-2.603697	-1.963630	-3.335967	1	2.800213	1.322913	-3.393470
1	-4.036738	-2.250848	-2.342929	1	4.223713	1.412464	-2.349241
1	-2.887450	-0.984236	-1.890197	1	2.800715	0.505155	-1.820662
6	4.106324	-2.207057	2.868161	6	-2.898369	2.862650	2.631219
1	4.043043	-3.227717	2.480210	1	-2.305247	3.592668	2.078755
1	5.162533	-1.918967	2.881366	1	-3.917955	3.252037	2.722898
1	3.744732	-2.212872	3.901274	1	-2.476552	2.785426	3.638266
6	3.309741	0.173824	2.590991	6	-3.637958	0.496855	2.864325
1	2.904075	0.177192	3.606931	1	-3.108118	0.415874	3.817284
1	4.324014	0.580587	2.639092	1	-4.657888	0.827377	3.090734
1	2.705022	0.842308	1.977546	1	-3.683821	-0.497009	2.418784
6	3.190149	-4.197371	-2.986040	6	-3.038137	4.318471	-3.217826
1	2.586568	-4.732493	-3.725391	1	-2.448303	4.784235	-4.013138
1	4.223117	-4.169887	-3.348130	1	-4.080022	4.276090	-3.551409
1	3.177001	-4.775434	-2.059132	1	-2.999068	4.971452	-2.342720
6	2.616122	-2.034102	-4.116674	6	-2.536206	2.060474	-4.180308
1	2.253601	-1.014232	-3.988250	1	-2.188223	1.046846	-3.981660

1	3.602794	-2.001413	-4.589464	1	-3.541883	2.002092	-4.607815
1	1.939067	-2.545905	-4.806368	1	-1.882433	2.501757	-4.938249
6	2.661898	3.956540	-2.640168	6	-2.917332	-3.867650	-2.493246
1	2.113054	4.835533	-2.289559	1	-2.425086	-4.743914	-2.061387
1	3.731459	4.180914	-2.571433	1	-3.998339	-4.037408	-2.453840
1	2.417345	3.800872	-3.695198	1	-2.625045	-3.797805	-3.545509
6	3.026083	1.475271	-2.340499	6	-3.160466	-1.354556	-2.383349
1	2.754812	1.290591	-3.383580	1	-2.826370	-1.255596	-3.420097
1	4.113485	1.583596	-2.289750	1	-4.253495	-1.404384	-2.388460
1	2.745729	0.597653	-1.755128	1	-2.865827	-0.455263	-1.839869
6	0.867950	4.506727	4.023486	6	-1.504910	-3.947915	4.320563
1	1.138447	5.492390	3.634419	1	-1.881534	-4.938908	4.051248
1	-0.040368	4.614336	4.622981	1	-0.633079	-4.078723	4.967535
1	1.662815	4.179290	4.700812	1	-2.272597	-3.441931	4.914240
6	0.308798	2.115590	3.459293	6	-0.648775	-1.731983	3.479627
1	-0.585975	2.151239	4.088765	1	0.227195	-1.785778	4.133912
1	0.139887	1.399610	2.651239	1	-0.389107	-1.144932	2.593412
1	1.139086	1.746933	4.068931	1	-1.441502	-1.201736	4.015966
6	-3.315034	2.797746	2.361600	6	2.959021	-2.928179	2.558800
1	-2.830354	3.540931	1.727057	1	2.359513	-3.650136	2.002586
1	-4.384370	3.030423	2.402737	1	3.981845	-3.314082	2.625638
1	-2.908569	2.906957	3.372064	1	2.553995	-2.872180	3.574086
6	-3.696567	0.393397	2.872385	6	3.688441	-0.561720	2.824218
1	-3.591901	-0.641004	2.546411	1	3.723282	0.439425	2.394123
1	-3.180211	0.502088	3.830407	1	3.172611	-0.498738	3.786208
1	-4.757600	0.596536	3.055197	1	4.713104	-0.891021	3.029983
6	-2.733406	1.333441	-4.321194	6	2.466000	-1.956449	-4.229106
1	-3.724241	1.113053	-4.731050	1	3.463393	-1.896021	-4.675378
1	-2.138048	1.780876	-5.122226	1	1.793007	-2.372493	-4.984485
1	-2.257581	0.396387	-4.033849	1	2.130967	-0.945545	-3.997134
6	-3.509164	3.593159	-3.565256	6	2.966893	-4.242125	-3.330733
1	-2.977651	4.053908	-4.403384	1	2.360846	-4.682657	-4.128204
1	-4.536421	3.393075	-3.886513	1	4.004162	-4.200996	-3.678518
1	-3.555181	4.322724	-2.753106	1	2.933818	-4.915826	-2.471292
1	5.171093	3.515116	1.769066	1	-5.600040	-2.873835	1.757715
1	-6.358693	-0.026309	-1.198508	1	6.304676	-0.833661	-1.275431
1	6.409387	-0.406299	-1.343352	1	-6.316093	0.847866	-1.186044
1	-5.264487	-3.219012	1.989292	1	5.605425	2.850863	1.805461

Side-on [Pd(IPr)$_2$]-O$_2$ scan Pd-O = 2.8 Å (OST)				Side-on [Pd(IPr)$_2$]-O$_2$ scan Pd-O = 3.0 Å (OST)			
46	-0.000125	0.000013	0.001356	46	0.016229	-0.006817	0.021507
8	-0.459024	-0.390238	-2.733053	8	-0.478799	-0.247164	-2.927569
8	0.459130	0.389622	-2.733084	8	0.294346	0.665977	-2.888797
7	-0.808518	-2.966525	0.278775	7	-0.685733	-2.992630	0.250055
7	1.229114	-2.802629	-0.320400	7	1.345414	-2.754604	-0.345983
7	0.808381	2.966379	0.280684	7	0.702631	2.977682	0.324799
7	-1.229206	2.802957	-0.318688	7	-1.334715	2.751581	-0.258643
6	0.155146	-2.028227	0.033128	6	0.243866	-2.018516	0.005655
6	-0.356240	-4.259541	0.075822	6	-0.186188	-4.268191	0.046912
1	-0.990829	-5.116219	0.228552	1	-0.788739	-5.147825	0.198976
6	0.932529	-4.156044	-0.299759	6	1.098424	-4.117786	-0.326654
1	1.668555	-4.905744	-0.533439	1	1.861907	-4.839948	-0.559381
6	-2.134019	-2.722975	0.754078	6	-2.027756	-2.798093	0.700132
6	-2.373220	-2.839681	2.130985	6	-2.299369	-2.977699	2.063881
6	-3.691345	-2.736036	2.566297	6	-3.631508	-2.928610	2.465679
1	-3.913498	-2.822410	3.623978	1	-3.880906	-3.067961	3.511407
6	-4.724114	-2.512381	1.665279	6	-4.644567	-2.691629	1.546042

6	-4.455828	-2.386406	0.312366	6	-4.343815	-2.498053	0.207626
1	-5.268453	-2.209238	-0.384048	1	-5.142454	-2.309425	-0.501198
6	-3.153791	-2.503532	-0.173418	6	-3.027029	-2.561647	-0.246049
6	-1.229847	-3.011664	3.107413	6	-1.174064	-3.153725	3.061055
1	-0.404216	-3.487423	2.570118	1	-0.340910	-3.634817	2.539582
6	-2.877878	-2.453314	-1.658414	6	-2.702389	-2.456038	-1.718283
1	-1.795516	-2.404342	-1.792340	1	-1.632776	-2.252192	-1.802381
6	2.551625	-2.337408	-0.601702	6	2.647163	-2.242840	-0.639872
6	3.046115	-2.465776	-1.904610	6	3.117153	-2.325189	-1.955092
6	4.384183	-2.138454	-2.126685	6	4.439494	-1.952379	-2.196628
1	4.795682	-2.233583	-3.125842	1	4.833187	-2.011953	-3.205729
6	5.181070	-1.670480	-1.097344	6	5.243239	-1.485850	-1.171695
6	4.656951	-1.522150	0.179739	6	4.741426	-1.381507	0.118693
1	5.286470	-1.136901	0.972480	1	5.375541	-0.995023	0.907203
6	3.340123	-1.871007	0.463430	6	3.440900	-1.774530	0.419652
6	2.184977	-2.944404	-3.055607	6	2.240911	-2.799127	-3.096325
1	1.144896	-2.941725	-2.717245	1	1.209390	-2.824931	-2.733523
6	2.784697	-1.797432	1.870578	6	2.904482	-1.736414	1.835732
1	1.765407	-1.403894	1.782277	1	1.873855	-1.368917	1.766253
6	-0.155261	2.028293	0.034291	6	-0.225896	2.008582	0.060563
6	0.356121	4.259540	0.078708	6	0.197979	4.257343	0.166142
1	0.990699	5.116088	0.232119	1	0.799971	5.133252	0.339997
6	-0.932614	4.156371	-0.297053	6	-1.089702	4.114395	-0.198991
1	-1.668625	4.906253	-0.530231	1	-1.857817	4.841648	-0.396776
6	2.134053	2.722390	0.755241	6	2.039962	2.776632	0.787054
6	3.153333	2.503180	-0.172840	6	3.064350	2.634196	-0.149505
6	4.455539	2.385326	0.312287	6	4.372982	2.560367	0.327293
1	5.267817	2.208304	-0.384561	1	5.188664	2.439456	-0.377851
6	4.724476	2.510459	1.665152	6	4.642715	2.657149	1.681997
6	3.692195	2.734017	2.566749	6	3.604883	2.804596	2.593047
1	3.914880	2.819799	3.624363	1	3.828113	2.868307	3.652123
6	2.373906	2.838292	2.132088	6	2.281272	2.859617	2.166349
6	2.876769	2.454276	-1.657768	6	2.787698	2.595515	-1.634010
1	1.794384	2.404974	-1.791288	1	1.704342	2.602359	-1.769459
6	1.231014	3.010193	3.109114	6	1.137340	2.946211	3.153580
1	0.405506	3.487005	2.572568	1	0.284345	3.391885	2.633862
6	-2.551691	2.337993	-0.600584	6	-2.648312	2.248945	-0.519916
6	-3.045876	2.467317	-1.903512	6	-3.187411	2.406596	-1.802484
6	-4.383937	2.140261	-2.126094	6	-4.517462	2.033262	-1.999550
1	-4.795227	2.236106	-3.125272	1	-4.962198	2.149268	-2.982074
6	-5.181093	1.671721	-1.097224	6	-5.263751	1.492066	-0.968499
6	-4.657258	1.522423	0.179868	6	-4.697878	1.322344	0.287719
1	-5.286990	1.136697	0.972214	1	-5.288165	0.882471	1.082110
6	-3.340440	1.870896	0.464078	6	-3.389490	1.717426	0.549422
6	-2.184449	2.946712	-3.053966	6	-2.383549	2.964543	-2.959396
1	-1.144494	2.944304	-2.715225	1	-1.330956	2.966277	-2.661875
6	-2.785239	1.796137	1.871243	6	-2.799702	1.626154	1.941695
1	-1.766022	1.402421	1.782787	1	-1.774163	1.256779	1.821886
6	1.576109	3.902106	4.297019	6	1.443421	3.825474	4.361368
1	1.969907	4.870368	3.974985	1	1.782592	4.820933	4.060798
1	0.680271	4.081130	4.898350	1	0.543919	3.941739	4.972676
1	2.316637	3.436331	4.954488	1	2.212844	3.384190	5.002375
6	0.741405	1.635548	3.567254	6	0.723224	1.536467	3.578755
1	1.516371	1.127574	4.150086	1	1.528022	1.053386	4.142062
1	-0.149678	1.732441	4.195944	1	-0.166078	1.570445	4.216361
1	0.495352	1.007582	2.705013	1	0.500909	0.919939	2.701243

6	3.381846	3.727461	-2.338509	6	3.359634	3.830578	-2.330175
1	2.922964	4.620817	-1.905084	1	2.951727	4.752744	-1.906139
1	4.467474	3.825402	-2.235228	1	4.449327	3.871799	-2.233474
1	3.145215	3.708290	-3.406796	1	3.118904	3.811032	-3.397509
6	3.462138	1.202430	-2.297470	6	3.310869	1.304160	-2.249677
1	3.206918	1.167950	-3.360681	1	3.070420	1.266802	-3.316257
1	4.552848	1.172107	-2.217289	1	4.396452	1.216623	-2.148947
1	3.061406	0.307289	-1.820068	1	2.854482	0.440902	-1.761069
6	-2.722461	3.186768	2.509535	6	-2.755587	3.004473	2.608283
1	-2.109716	3.881880	1.932329	1	-2.170849	3.726831	2.035874
1	-3.727046	3.613855	2.599059	1	-3.768008	3.405343	2.726704
1	-2.294139	3.118963	3.514618	1	-2.306448	2.925005	3.603379
6	-3.554843	0.844763	2.773633	6	-3.528177	0.642690	2.843706
1	-3.030729	0.745256	3.728151	1	-2.983017	0.542982	3.786240
1	-4.563035	1.212290	2.995627	1	-4.539903	0.983300	3.091109
1	-3.635262	-0.147861	2.329448	1	-3.593840	-0.345289	2.387161
6	-2.553647	4.374091	-3.463958	6	-2.798148	4.402188	-3.281728
1	-1.907245	4.719280	-4.276576	1	-2.195783	4.799653	-4.104286
1	-3.589528	4.417702	-3.815428	1	-3.849341	4.438740	-3.585046
1	-2.456496	5.077635	-2.633883	1	-2.677948	5.068472	-2.424804
6	-2.275325	2.015436	-4.263028	6	-2.507024	2.098870	-4.213700
1	-2.069733	0.981502	-3.984708	1	-2.295262	1.051185	-3.998976
1	-3.267156	2.053008	-4.723818	1	-3.511153	2.159364	-4.644613
1	-1.548821	2.317774	-5.023023	1	-1.802765	2.443438	-4.976616
6	-3.383842	-3.725492	-2.340329	6	-2.995751	-3.783726	-2.419792
1	-2.925194	-4.619538	-1.908056	1	-2.430795	-4.605859	-1.971504
1	-4.469476	-3.823056	-2.236742	1	-4.060120	-4.032725	-2.355076
1	-3.147616	-3.705258	-3.408691	1	-2.724942	-3.724528	-3.478582
6	-3.462884	-1.200426	-2.296381	6	-3.425901	-1.296319	-2.387304
1	-3.208143	-1.164770	-3.359677	1	-3.118181	-1.218555	-3.434139
1	-4.553532	-1.169601	-2.215594	1	-4.513059	-1.421197	-2.374294
1	-3.061407	-0.306089	-1.818051	1	-3.183800	-0.357329	-1.888572
6	-1.573881	-3.904889	4.294639	6	-1.541373	-4.039846	4.246170
1	-1.967170	-4.873109	3.971853	1	-1.933242	-5.008379	3.922385
1	-0.677687	-4.083887	4.895447	1	-0.656189	-4.219076	4.862862
1	-2.314463	-3.440213	4.952828	1	-2.290603	-3.567851	4.889238
6	-0.741031	-1.637070	3.566518	6	-0.685855	-1.780073	3.525410
1	0.150218	-1.733870	4.194990	1	0.204670	-1.878862	4.154538
1	-0.495483	-1.008368	2.704654	1	-0.440822	-1.145118	2.667886
1	-1.516219	-1.129990	4.149838	1	-1.462076	-1.276582	4.110077
6	2.722183	-3.188589	2.507751	6	2.885481	-3.135745	2.457610
1	2.109740	-3.883392	1.929852	1	2.277023	-3.837710	1.884472
1	3.726864	-3.615479	2.597120	1	3.900937	-3.540950	2.523478
1	2.293655	-3.121725	3.512813	1	2.474881	-3.089067	3.471202
6	3.553911	-0.846550	2.773813	6	3.663020	-0.777727	2.739969
1	3.634128	0.146418	2.330379	1	3.715305	0.221488	2.306408
1	3.029639	-0.747909	3.728334	1	3.148959	-0.701168	3.702004
1	4.562170	-1.213961	2.995693	1	4.681908	-1.125130	2.944898
6	2.276669	-2.012713	-4.264305	6	2.284000	-1.840151	-4.285876
1	3.268477	-2.050975	-4.725089	1	3.265366	-1.845032	-4.769998
1	1.549934	-2.314146	-5.024437	1	1.546442	-2.140775	-5.035808
1	2.072012	-0.978706	-3.985609	1	2.064274	-0.817282	-3.979228
6	2.553798	-4.371741	-3.466081	6	2.628863	-4.209643	-3.544572
1	1.907638	-4.716294	-4.279167	1	1.974615	-4.549043	-4.353375
1	3.589823	-4.415577	-3.817102	1	3.659250	-4.226685	-3.914127
1	2.455996	-5.075656	-2.636404	1	2.557776	-4.931981	-2.728218

1	-5.744945	-2.431050	2.024832		1	-5.676616	-2.652468	1.879799
1	6.216198	-1.407226	-1.290010		1	6.266510	-1.188688	-1.378207
1	-6.216223	1.408750	-1.290272		1	-6.291578	1.190616	-1.143168
1	5.745444	2.428592	2.024196		1	5.667984	2.611853	2.035162

Side-on [Pd(IPr)$_2$]-O$_2$ scan Pd-O = 3.2 Å (OST)

46	0.010095	-0.002349	0.046873
8	-0.349733	-0.354732	-3.113223
8	0.184787	0.711769	-3.067508
7	-0.548869	-3.014200	0.200799
7	1.476519	-2.678712	-0.369906
7	0.554537	2.998481	0.366023
7	-1.473930	2.692106	-0.211564
6	0.339863	-1.996454	-0.017565
6	0.007020	-4.263351	-0.018027
1	-0.558241	-5.170540	0.113977
6	1.287610	-4.051356	-0.375200
1	2.083759	-4.736605	-0.609469
6	-1.897556	-2.886015	0.655548
6	-2.158263	-3.100173	2.016331
6	-3.490404	-3.120076	2.420456
1	-3.730675	-3.288504	3.464078
6	-4.515172	-2.914217	1.506338
6	-4.225970	-2.680390	0.171770
1	-5.033533	-2.512963	-0.532373
6	-2.908383	-2.675194	-0.284138
6	-1.025010	-3.236244	3.010608
1	-0.165037	-3.654369	2.478882
6	-2.590414	-2.520835	-1.753069
1	-1.528840	-2.277338	-1.831265
6	2.759554	-2.106133	-0.633216
6	3.262541	-2.161098	-1.938066
6	4.566040	-1.712379	-2.151444
1	4.983943	-1.748477	-3.151897
6	5.318802	-1.198636	-1.110895
6	4.787217	-1.131474	0.169899
1	5.382739	-0.712358	0.971650
6	3.507308	-1.603630	0.444760
6	2.444238	-2.686770	-3.099935
1	1.405185	-2.761724	-2.766751
6	2.952388	-1.618370	1.854430
1	1.909848	-1.286799	1.780962
6	-0.331744	1.993060	0.091044
6	-0.005615	4.257010	0.228242
1	0.559066	5.155685	0.410840
6	-1.287878	4.063294	-0.132552
1	-2.088388	4.759082	-0.314615
6	1.907876	2.846875	0.798520
6	2.914241	2.747712	-0.162631
6	4.235388	2.719119	0.283095
1	5.038811	2.632367	-0.440951
6	4.532187	2.817489	1.632018
6	3.511119	2.921428	2.567950
1	3.757351	2.988273	3.621714
6	2.176672	2.929429	2.172525
6	2.601477	2.711337	-1.639888
1	1.516249	2.650290	-1.746432

6	1.051237	2.964556	3.184356
1	0.178537	3.404908	2.693250
6	-2.766310	2.139866	-0.477291
6	-3.316117	2.299902	-1.755018
6	-4.630576	1.876934	-1.955857
1	-5.082772	1.993331	-2.934943
6	-5.350679	1.286647	-0.933298
6	-4.773758	1.115888	0.317803
1	-5.343469	0.637710	1.105009
6	-3.481359	1.558314	0.583803
6	-2.538534	2.908350	-2.904234
1	-1.486558	2.950411	-2.608099
6	-2.881840	1.460573	1.971563
1	-1.847804	1.118647	1.839090
6	1.362458	3.816531	4.410021
1	1.676082	4.826570	4.131129
1	0.472767	3.897356	5.041022
1	2.152563	3.373022	5.023709
6	0.676048	1.534942	3.579024
1	1.499281	1.058702	4.120694
1	-0.206122	1.530885	4.227289
1	0.459114	0.933355	2.689402
6	3.076648	3.990408	-2.329363
1	2.623103	4.878454	-1.879625
1	4.163840	4.097928	-2.258220
1	2.810147	3.972541	-3.390619
6	3.186570	1.465022	-2.290857
1	2.924311	1.434170	-3.352491
1	4.277521	1.439427	-2.216528
1	2.792977	0.567977	-1.808345
6	-2.867763	2.828127	2.661395
1	-2.300582	3.573861	2.101811
1	-3.889046	3.203346	2.788012
1	-2.415832	2.741515	3.654556
6	-3.582111	0.446952	2.862654
1	-3.029360	0.346242	3.800592
1	-4.599738	0.761550	3.120341
1	-3.628473	-0.535791	2.392747
6	-3.013012	4.331655	-3.206988
1	-2.429273	4.764299	-4.025250
1	-4.065529	4.329533	-3.508032
1	-2.917990	4.990971	-2.341549
6	-2.628089	2.054865	-4.169704
1	-2.375734	1.013636	-3.968449
1	-3.634305	2.080314	-4.599215
1	-1.938749	2.436401	-4.928571
6	-2.837329	-3.838732	-2.489697
1	-2.244803	-4.652238	-2.061580
1	-3.892450	-4.126413	-2.434081
1	-2.567417	-3.742760	-3.546047
6	-3.354096	-1.369005	-2.389954
1	-3.052449	-1.254500	-3.435221
1	-4.436485	-1.529657	-2.377552
1	-3.142245	-0.435762	-1.866760
6	-1.339625	-4.172282	4.172142
1	-1.672964	-5.153738	3.822751

1	-0.445300	-4.314508	4.785350
1	-2.115663	-3.763229	4.826538
6	-0.617895	-1.847997	3.508521
1	0.274090	-1.909785	4.140257
1	-0.405120	-1.182439	2.665615
1	-1.423970	-1.401949	4.099428
6	2.978275	-3.032469	2.442746
1	2.403177	-3.743858	1.847603
1	4.007631	-3.400523	2.511390
1	2.555689	-3.024521	3.452410
6	3.667476	-0.660520	2.794426
1	3.690560	0.352895	2.392517
1	3.141267	-0.631548	3.752470
1	4.695199	-0.980017	3.000611
6	2.474782	-1.737411	-4.297611
1	3.465980	-1.706547	-4.760294
1	1.767160	-2.074217	-5.060773
1	2.208329	-0.721484	-4.006287
6	2.916566	-4.078470	-3.526194
1	2.306539	-4.453932	-4.353407
1	3.957847	-4.044812	-3.862419
1	2.856346	-4.800722	-2.709110
1	-5.547348	-2.929255	1.841684
1	6.326109	-0.839593	-1.296615
1	-6.366379	0.947865	-1.110552
1	5.566325	2.808394	1.961448

trans-[Ir(Cl)(CO)(PPh3)2]				**_trans_-[Ir(Cl)(CO)(PPh3)2]** at PBE0/BSI level			
77	0.001725	0.118516	-0.131339	77	0.000007	0.121609	-0.000446
17	-0.000856	-2.262218	0.039580	17	-0.000122	-2.267469	-0.000098
8	0.008025	3.069604	-0.436753	8	0.000054	3.089573	-0.001284
6	0.004511	1.923118	-0.310127	6	0.000041	1.935875	-0.000923
15	2.320958	0.016615	-0.025534	15	2.336928	0.014899	0.011235
15	-2.317263	0.018404	-0.039524	15	-2.336913	0.014918	-0.011514
6	2.851745	-0.926863	1.443069	6	2.960915	-1.041236	1.369534
6	3.984890	-1.735629	1.449498	6	4.083463	-1.856797	1.239641
1	4.570009	-1.857814	0.544644	1	4.604339	-1.919788	0.290386
6	4.354033	-2.402005	2.611907	6	4.527522	-2.607087	2.322389
1	5.231773	-3.039558	2.609947	1	5.396317	-3.247540	2.211164
6	3.598710	-2.259833	3.769097	6	3.859377	-2.543688	3.538696
1	3.888362	-2.784188	4.673728	1	4.207964	-3.132117	4.381219
6	2.464459	-1.454927	3.763990	6	2.735136	-1.736040	3.670612
1	1.865140	-1.350557	4.662272	1	2.201438	-1.693949	4.614366
6	2.086310	-0.796121	2.603436	6	2.280928	-0.994771	2.588710
1	1.186837	-0.187316	2.576789	1	1.385654	-0.385240	2.673382
6	3.185639	1.617534	0.156825	6	3.219013	1.605879	0.260744
6	3.210264	-0.736493	-1.435125	6	3.139702	-0.626249	-1.511804
6	4.540133	-0.399919	-1.701566	6	4.452121	-0.265927	-1.833019
1	5.044931	0.340255	-1.089664	1	4.997179	0.423070	-1.196252
6	5.213467	-1.000401	-2.757017	6	5.060032	-0.774364	-2.973852
1	6.245341	-0.732799	-2.958683	1	6.078261	-0.486045	-3.213895
6	4.564924	-1.936363	-3.554462	6	4.364118	-1.643402	-3.806042
1	5.091386	-2.402529	-4.380842	1	4.838597	-2.037323	-4.699057
6	3.241488	-2.270019	-3.294595	6	3.058994	-2.002239	-3.493132
1	2.731063	-2.998661	-3.915335	1	2.510098	-2.679744	-4.138870
6	2.561688	-1.672871	-2.240786	6	2.445052	-1.497186	-2.353364

1	1.532556	-1.938869	-2.027859
6	-2.997370	-0.417237	1.603335
6	-4.268605	0.014289	1.990662
1	-4.853067	0.642992	1.327207
6	-4.781447	-0.347570	3.229705
1	-5.768500	-0.006064	3.523268
6	-4.030651	-1.139462	4.090451
1	-4.431530	-1.418876	5.059247
6	-2.765198	-1.568586	3.709204
1	-2.174657	-2.186922	4.376957
6	-2.245534	-1.209039	2.472605
1	-1.262802	-1.551821	2.169334
6	-3.028493	-1.200828	-1.193179
6	-2.405646	-1.359491	-2.431949
1	-1.496665	-0.803566	-2.642148
6	-2.935411	-2.234789	-3.368893
1	-2.446498	-2.356672	-4.329518
6	-4.078468	-2.967507	-3.068524
1	-4.485867	-3.660477	-3.797245
6	-4.690967	-2.822673	-1.829936
1	-5.574726	-3.403669	-1.588429
6	-4.170169	-1.939469	-0.892289
1	-4.643770	-1.836320	0.077811
6	-3.218264	1.559688	-0.433856
6	-3.029802	2.667088	0.396657
1	-2.372026	2.591912	1.256778
6	-3.678276	3.861579	0.126038
1	-3.522964	4.716455	0.775138
6	-4.516084	3.965274	-0.979884
1	-5.019454	4.902186	-1.193738
6	-4.703741	2.868915	-1.810148
1	-5.355905	2.944519	-2.673819
6	-4.059427	1.666452	-1.539182
1	-4.213222	0.810181	-2.186451
6	3.114319	2.529523	-0.899111
1	2.563621	2.273102	-1.798749
6	3.743020	3.760755	-0.802629
1	3.678838	4.462979	-1.626676
6	4.444892	4.096916	0.350615
1	4.933184	5.062655	0.426944
6	3.890437	1.956922	1.309446
1	3.954074	1.253708	2.132305
6	4.516034	3.195538	1.403685
1	5.062139	3.452629	2.305159

[Ir(Cl)(CO)(PPh$_3$)$_2$(η^2-O$_2$)]

77	0.003775	-0.108668	0.005361
17	0.057482	0.223447	2.384404
8	-0.046686	-3.105982	-0.002881
6	-0.032205	-1.959864	0.038037
8	0.077152	1.746759	-0.797702
8	-0.056162	0.766551	-1.795196
15	-2.355183	0.020044	-0.046115
15	2.357095	0.013340	-0.028685
6	-3.242005	-0.563053	1.432525
6	-4.442820	0.037592	1.813568
1	-4.816775	0.895187	1.265194

1	1.430706	-1.788479	-2.104933
6	-3.138936	-0.625247	1.512329
6	-4.451144	-0.264625	1.834047
1	-4.996479	0.424042	1.197175
6	-5.058487	-0.772334	2.975509
1	-6.076553	-0.483759	3.215937
6	-4.362222	-1.640981	3.807811
1	-4.836261	-2.034347	4.701308
6	-3.057313	-2.000151	3.494382
1	-2.508148	-2.677371	4.140194
6	-2.443934	-1.495802	2.354000
1	-1.429751	-1.787359	2.105225
6	-2.961616	-1.042048	-1.368839
6	-2.282621	-0.995911	-2.588573
1	-1.387621	-0.386140	-2.674263
6	-2.737490	-1.737771	-3.669792
1	-2.204586	-1.695916	-4.614007
6	-3.861367	-2.545726	-3.536605
1	-4.210458	-3.134624	-4.378597
6	-4.528486	-2.608824	-2.319720
1	-5.396975	-3.249523	-2.207511
6	-4.083786	-1.857908	-1.237673
1	-4.603847	-1.920648	-0.287963
6	-3.219036	1.605804	-0.261566
6	-3.090002	2.595027	0.717512
1	-2.487001	2.407369	1.600558
6	-3.727783	3.817077	0.568656
1	-3.617766	4.577189	1.334782
6	-4.496647	4.069821	-0.562850
1	-4.991858	5.028049	-0.680839
6	-4.624988	3.093756	-1.541312
1	-5.222769	3.284485	-2.426587
6	-3.991012	1.864109	-1.393072
1	-4.101480	1.104820	-2.159358
6	3.090306	2.594647	-0.718830
1	2.487524	2.406619	-1.601952
6	3.728132	3.816723	-0.570347
1	3.618372	4.576492	-1.336845
6	4.496710	4.069936	0.561247
1	4.991944	5.028187	0.678925
6	3.990717	1.864641	1.392340
1	4.100925	1.105663	2.158991
6	4.624732	3.094316	1.540192
1	5.222288	3.285412	2.425542

[Ir(Cl)(CO)(PPh$_3$)$_2$(η^2-O$_2$)] at PBE0/BSI level

77	0.000076	-0.110989	0.016368
17	0.055164	0.034209	2.418684
8	-0.054830	-3.102297	-0.201568
6	-0.038184	-1.961542	-0.081840
8	0.074807	1.799994	-0.646675
8	-0.059424	0.896309	-1.714966
15	-2.377537	0.023133	-0.040588
15	2.369985	0.015638	-0.021250
6	-3.282580	-0.656423	1.394150
6	-4.486783	-0.082066	1.807640
1	-4.860006	0.808911	1.314384

6	-5.153881	-0.455777	2.899434	6	-5.204611	-0.642943	2.856411
1	-6.084156	0.018878	3.192532	1	-6.136552	-0.186510	3.173035
6	-4.672214	-1.548240	3.610055	6	-4.728086	-1.778587	3.499619
1	-5.226634	-1.929979	4.460899	1	-5.287809	-2.213082	4.321447
6	-3.473058	-2.143854	3.237824	6	-3.526887	-2.349326	3.096941
1	-3.084216	-2.986160	3.799351	1	-3.140766	-3.225641	3.606286
6	-2.755941	-1.651565	2.156742	6	-2.802990	-1.789291	2.053133
1	-1.809192	-2.104120	1.891273	1	-1.854372	-2.226432	1.768374
6	-3.083194	-0.934156	-1.416455	6	-3.094346	-0.844442	-1.482382
6	-2.925926	1.726787	-0.263862	6	-2.952140	1.745670	-0.155415
6	-3.899253	2.070188	-1.198166	6	-3.906397	2.153309	-1.085020
1	-4.308734	1.314393	-1.859419	1	-4.303911	1.445487	-1.804288
6	-4.340936	3.385930	-1.281789	6	-4.346618	3.472627	-1.092694
1	-5.097406	3.653944	-2.011598	1	-5.087511	3.787449	-1.820115
6	-3.813921	4.351526	-0.434493	6	-3.838366	4.381449	-0.174183
1	-4.159271	5.377919	-0.502143	1	-4.182289	5.410716	-0.182606
6	-2.838860	4.006694	0.496551	6	-2.883227	3.974898	0.752369
1	-2.420101	4.762234	1.152376	1	-2.477939	4.685451	1.464860
6	-2.386818	2.699336	0.580772	6	-2.432598	2.663583	0.760564
1	-1.617968	2.426548	1.296387	1	-1.677847	2.347212	1.473427
6	3.171725	-1.499100	0.578893	6	3.201250	-1.537186	0.472935
6	4.202447	-2.113177	-0.131059	6	4.228570	-2.095994	-0.288196
1	4.534336	-1.694743	-1.074714	1	4.550144	-1.614616	-1.205054
6	4.797769	-3.265099	0.369680	6	4.839005	-3.274956	0.124669
1	5.595711	-3.742691	-0.188855	1	5.633495	-3.705575	-0.475822
6	4.372835	-3.802166	1.577780	6	4.434811	-3.897924	1.298074
1	4.839153	-4.701877	1.965297	1	4.913096	-4.818102	1.617511
6	3.346653	-3.188437	2.288511	6	3.413407	-3.342033	2.060970
1	3.010301	-3.606325	3.231253	1	3.091759	-3.825400	2.977433
6	2.742145	-2.042409	1.793443	6	2.793358	-2.169359	1.652486
1	1.939111	-1.560749	2.344648	1	1.993201	-1.737661	2.247481
6	3.040525	1.357527	0.986897	6	3.070261	1.294091	1.077640
6	2.526991	2.646268	0.818395	6	2.552138	2.590844	1.009667
1	1.723029	2.806578	0.107248	1	1.732288	2.798165	0.329250
6	3.048669	3.693659	1.562621	6	3.088595	3.588592	1.810878
1	2.646881	4.692987	1.433283	1	2.681961	4.593072	1.756938
6	4.073907	3.466315	2.474812	6	4.133973	3.304808	2.683262
1	4.474476	4.288946	3.058049	1	4.546207	4.088022	3.311284
6	4.582388	2.185148	2.641547	6	4.647234	2.016524	2.752478
1	5.379795	2.002476	3.353958	1	5.460367	1.788350	3.433638
6	4.068598	1.128566	1.899333	6	4.119004	1.010198	1.951915
1	4.464536	0.128668	2.035804	1	4.522458	0.005777	2.014689
6	3.039012	0.271573	-1.690166	6	3.042068	0.387909	-1.673911
6	2.472084	-0.415284	-2.764570	6	2.474805	-0.228845	-2.790796
1	1.596235	-1.033259	-2.605683	1	1.602574	-0.861330	-2.673016
6	3.021098	-0.290325	-4.032071	6	3.017058	-0.019267	-4.050715
1	2.576071	-0.822674	-4.865701	1	2.570056	-0.499642	-4.914615
6	4.125849	0.529299	-4.236664	6	4.116700	0.817343	-4.207977
1	4.547080	0.632473	-5.231235	1	4.532950	0.986600	-5.195775
6	4.684492	1.223302	-3.170866	6	4.675927	1.443362	-3.101367
1	5.541770	1.868758	-3.329118	1	5.529238	2.102744	-3.220245
6	4.144021	1.095883	-1.897261	6	4.142164	1.230145	-1.835841
1	4.576202	1.640330	-1.064826	1	4.578420	1.723438	-0.974069
6	-2.586891	-0.729326	-2.708585	6	-2.583092	-0.562256	-2.754537
1	-1.788567	-0.008618	-2.859884	1	-1.781394	0.164013	-2.852880
6	-3.118102	-1.447247	-3.770189	6	-3.102711	-1.210738	-3.866243

1	-2.733933	-1.283949	-4.771568	1	-2.705240	-0.985937	-4.850588
6	-4.133050	-2.374165	-3.554599	6	-4.122126	-2.146508	-3.722281
1	-4.541867	-2.935901	-4.387995	1	-4.521676	-2.654139	-4.594242
6	-4.100422	-1.863200	-1.201289	6	-4.116831	-1.782981	-1.340810
1	-4.483550	-2.027642	-0.200534	1	-4.514172	-2.010296	-0.357945
6	-4.620667	-2.581858	-2.271316	6	-4.625630	-2.432118	-2.460257
1	-5.409583	-3.305912	-2.097811	1	-5.418261	-3.163446	-2.341461

[V(N[tBu]Ar)3]				[V(N[tBu]Ar)3] at PBE0/BSI level			
6	5.592651	0.467063	-2.220236	6	5.636584	0.141724	-2.304168
6	5.142638	0.953391	0.209028	6	5.258382	0.769577	0.104923
6	4.791673	0.281940	-0.963531	6	4.836242	0.081468	-1.033420
6	1.871082	2.936253	-1.951533	6	1.903219	2.878161	-2.198151
6	4.775729	1.536748	2.634115	6	4.982128	1.483712	2.505850
6	4.418399	0.783677	1.385381	6	4.542323	0.706328	1.297381
6	3.687251	-0.563613	-0.946337	6	3.670894	-0.676981	-0.964108
6	0.707804	2.854270	-1.008662	6	0.767614	2.880822	-1.216918
6	-0.357470	3.732127	-1.094930	6	-0.237797	3.828745	-1.287088
6	3.323400	-0.079594	1.377821	6	3.385708	-0.071451	1.341491
6	2.932155	-0.752909	0.217667	6	2.927203	-0.770217	0.220003
6	0.703666	1.897475	0.016391	6	0.732581	1.943369	-0.172419
6	0.683919	-0.666745	-3.067748	6	0.523898	-0.889444	-3.080567
6	-1.407233	3.685692	-0.159884	6	-1.265710	3.862815	-0.328189
6	-2.525470	4.681819	-0.263949	6	-2.311970	4.937741	-0.411488
6	-0.387851	1.761144	0.916416	6	-0.332153	1.898512	0.766194
6	2.708519	-3.621004	-0.659296	6	2.638205	-3.678138	-0.467855
6	-1.435473	0.578350	-3.441166	6	-1.650743	0.243587	-3.492350
6	-1.428153	2.715435	0.824683	6	-1.319449	2.908903	0.672438
6	-0.821422	-0.684753	-2.828235	6	-0.969587	-0.925846	-2.770979
6	1.834142	-2.959035	0.409183	6	1.798332	-2.931833	0.575738
6	2.412891	-3.261092	1.794364	6	2.411635	-3.160287	1.962374
6	-0.797152	1.508281	3.875617	6	-0.591902	1.857660	3.751964
6	-1.423253	-1.921943	-3.498091	6	-1.551898	-2.244189	-3.292269
6	-1.058814	0.361145	2.898019	6	-0.978036	0.666761	2.869228
6	0.424843	-3.531645	0.311708	6	0.385129	-3.505027	0.555809
6	-0.463686	-0.921381	3.477501	6	-0.431172	-0.607843	3.513520
6	-3.168619	0.315605	-0.800273	6	-3.265463	0.241279	-0.754969
6	-2.365836	-0.830492	-0.899522	6	-2.448071	-0.899363	-0.790106
6	-2.563369	0.142058	2.703393	6	-2.504594	0.531028	2.781860
6	-5.278473	1.501488	-0.131766	6	-5.420007	1.423032	-0.217327
6	-4.451066	0.256630	-0.273762	6	-4.552028	0.196257	-0.232304
6	-2.890321	-2.045633	-0.454012	6	-2.959573	-2.091297	-0.268569
6	-4.945238	-0.976060	0.160471	6	-5.028622	-1.013260	0.279141
6	-4.176869	-2.131816	0.082240	6	-4.244369	-2.161655	0.274007
6	-4.698944	-3.446428	0.586321	6	-4.754374	-3.451107	0.853668
7	1.731310	-1.505556	0.200196	7	1.701780	-1.488477	0.268847
7	-0.346857	0.603482	1.644825	7	-0.327167	0.777882	1.559771
7	-1.030891	-0.752448	-1.372234	7	-1.123047	-0.841267	-1.303671
23	0.162270	-0.434653	0.076129	23	0.126999	-0.412213	0.080543
1	-0.234130	-3.080109	1.063675	1	-0.251326	-3.012400	1.301115
1	0.001991	-3.335598	-0.676964	1	-0.068437	-3.370865	-0.429659
1	0.431076	-4.611121	0.486400	1	0.398753	-4.572842	0.792824
1	2.744685	-4.703716	-0.503697	1	2.657060	-4.749159	-0.241706
1	2.305231	-3.431569	-1.658430	1	2.217047	-3.548410	-1.469293
1	3.732387	-3.240894	-0.622461	1	3.670500	-3.319677	-0.478419
1	1.780236	-2.826355	2.572867	1	1.808538	-2.674400	2.734399
1	2.477552	-4.341078	1.960926	1	2.461516	-4.230812	2.186827

1	3.417560	-2.842003	1.896594	1	3.426819	-2.758122	2.015581
1	2.716892	-0.204007	2.269925	1	2.797705	-0.123236	2.252807
1	5.992219	1.631589	0.200335	1	6.161771	1.373014	0.057634
1	3.374599	-1.063431	-1.856592	1	3.313293	-1.197434	-1.846508
1	6.439538	-0.227363	-2.249667	1	6.421352	-0.623018	-2.307592
1	4.984521	0.280517	-3.108577	1	5.007010	-0.032246	-3.180152
1	5.998083	1.479757	-2.289463	1	6.126615	1.111630	-2.422902
1	5.709406	2.089991	2.513198	1	6.016282	1.821728	2.407877
1	3.990337	2.254310	2.893194	1	4.354766	2.370144	2.649512
1	4.890289	0.859295	3.485316	1	4.906211	0.881374	3.415325
1	2.719515	2.354990	-1.583551	1	2.794566	2.410262	-1.773497
1	1.596928	2.539723	-2.935361	1	1.634204	2.314337	-3.098684
1	2.192331	3.971072	-2.095943	1	2.157370	3.893276	-2.513002
1	-0.366727	4.497662	-1.865965	1	-0.212718	4.585689	-2.066452
1	-2.145458	5.704996	-0.183272	1	-1.859571	5.929534	-0.309905
1	-3.029324	4.601645	-1.232869	1	-2.821292	4.914801	-1.380290
1	-3.270475	4.533235	0.520098	1	-3.065400	4.829118	0.371448
1	-4.776483	2.361677	-0.579330	1	-4.832610	2.325612	-0.400910
1	-6.254473	1.388859	-0.613525	1	-6.192359	1.367085	-0.992339
1	-5.463519	1.731198	0.923308	1	-5.932054	1.537693	0.742543
1	-4.517156	-4.248473	-0.134539	1	-4.551697	-4.294367	0.187248
1	-4.203168	-3.730864	1.520698	1	-4.269691	-3.670867	1.811129
1	-5.772726	-3.400615	0.780137	1	-5.831652	-3.410005	1.029432
1	-5.947054	-1.030873	0.579706	1	-6.031774	-1.056366	0.697098
1	-2.275026	-2.935702	-0.535134	1	-2.337329	-2.979882	-0.299349
1	-2.751528	1.267985	-1.104803	1	-2.862922	1.179241	-1.122545
1	1.637355	1.388334	0.259460	1	1.642076	1.381658	0.051131
1	-2.268596	2.671535	1.504733	1	-2.138074	2.934666	1.379707
1	-0.925137	-1.162682	4.439113	1	-0.848208	-0.742009	4.515895
1	-0.633536	-1.762815	2.799025	1	-0.697675	-1.486922	2.918536
1	0.614480	-0.812587	3.618596	1	0.658120	-0.563883	3.588490
1	0.278203	1.628942	4.033352	1	0.495944	1.921544	3.844785
1	-1.191202	2.456857	3.503692	1	-0.950346	2.804535	3.341478
1	-1.268740	1.300340	4.840525	1	-1.018354	1.741044	4.752801
1	-3.026713	-0.137359	3.655110	1	-2.917645	0.329336	3.775915
1	-3.071944	1.033836	2.334924	1	-2.986778	1.433514	2.402582
1	-2.744238	-0.660371	1.984496	1	-2.780758	-0.294373	2.120975
1	-0.965455	-2.831959	-3.098843	1	-1.053779	-3.097385	-2.821818
1	-2.500908	-1.976041	-3.321542	1	-2.622584	-2.313491	-3.081759
1	-1.255370	-1.896126	-4.579296	1	-1.413823	-2.321285	-4.375624
1	-1.042844	1.472251	-2.946992	1	-1.266580	1.199085	-3.122825
1	-1.196474	0.634222	-4.508126	1	-1.458711	0.185124	-4.568886
1	-2.523623	0.578754	-3.343035	1	-2.733639	0.226178	-3.346681
1	1.148888	-1.557491	-2.638821	1	1.037856	-1.719031	-2.588479
1	0.903389	-0.632509	-4.138928	1	0.692755	-0.961216	-4.159300
1	1.140884	0.210099	-2.598437	1	0.972366	0.045146	-2.727700
[V(N[^{t}Bu]Ar)$_3$(η^2-O$_2$)]				**[V(N[^{t}Bu]Ar)$_3$(η^2-O$_2$)]** at PBE0/BSI level			
7	-1.520566	1.027101	-0.888757	7	-1.505555	1.000020	-0.963048
7	1.120377	-0.313865	-1.612998	7	1.462461	0.256161	-1.336572
7	-0.958006	-1.763844	-0.001569	7	-0.581092	-1.850351	-0.576810
6	-1.589480	1.313942	0.504932	6	-1.913068	0.946406	0.403303
6	-2.678236	0.889147	1.271139	6	-3.047140	0.223410	0.791119
6	-2.770806	1.200777	2.620140	6	-3.486115	0.226994	2.108040
6	-1.755318	1.967962	3.200039	6	-2.772569	0.977424	3.048649
6	-0.671946	2.418111	2.455384	6	-1.648037	1.711245	2.690314
6	-0.593532	2.075983	1.103207	6	-1.220504	1.681638	1.359404

6	-2.370911	1.920456	-1.767043	6	-2.311055	1.956897	-1.828924
6	1.766932	0.783579	-0.976218	6	1.784648	1.250035	-0.364505
6	1.780015	2.044594	-1.574751	6	1.712318	2.610111	-0.682736
6	2.406950	3.122767	-0.959026	6	2.051594	3.585593	0.248558
6	3.037998	2.917229	0.268738	6	2.470765	3.180975	1.517980
6	3.050791	1.665655	0.878837	6	2.555786	1.834756	1.860433
6	2.399475	0.605221	0.251643	6	2.201484	0.874886	0.911013
6	1.965637	-1.086098	-2.575920	6	2.592536	-0.130309	-2.247347
6	0.114888	-1.835309	0.938785	6	0.277608	-2.023095	0.554208
6	1.195565	-2.704660	0.744175	6	1.507452	-2.688707	0.443977
6	2.209217	-2.822158	1.685459	6	2.306979	-2.927392	1.554066
6	2.133428	-2.055732	2.852508	6	1.862176	-2.492751	2.806510
6	1.071906	-1.187633	3.075443	6	0.646445	-1.835601	2.951228
6	0.070828	-1.082963	2.107482	6	-0.133417	-1.599337	1.815336
6	-1.959775	-2.869569	0.151762	6	-1.367610	-3.088753	-0.919275
6	-3.918199	0.700181	3.448603	6	-4.697119	-0.559449	2.523934
6	0.390602	3.279066	3.073618	6	-0.914547	2.547690	3.700111
6	-2.834914	3.161828	-0.997839	6	-3.172503	2.891186	-0.969264
6	-3.602775	1.149842	-2.241493	6	-3.239193	1.167319	-2.754336
6	-1.550974	2.423211	-2.955285	6	-1.373242	2.854384	-2.639172
6	2.417098	4.474941	-1.611654	6	1.987211	5.044780	-0.105168
6	3.770195	1.443735	2.177969	6	3.045154	1.410304	3.216445
6	2.190776	-0.241386	-3.831984	6	2.861029	1.002478	-3.243114
6	3.313510	-1.432396	-1.939999	6	3.860482	-0.405858	-1.433045
6	1.264033	-2.382788	-2.979869	6	2.238640	-1.392352	-3.036925
6	3.378691	-3.732671	1.445637	6	3.625370	-3.636321	1.419836
6	0.989851	-0.363758	4.327311	6	0.155077	-1.407660	4.305116
6	-3.359176	-2.389114	-0.236006	6	-2.743159	-2.716406	-1.479282
6	-2.043431	-3.339346	1.608427	6	-1.624616	-3.947767	0.326481
6	-1.552353	-4.059468	-0.725077	6	-0.600536	-3.938715	-1.941512
1	-3.452507	0.302702	0.793424	1	-3.586860	-0.341931	0.040853
1	-1.817175	2.220061	4.255844	1	-3.109628	0.990744	4.082689
1	0.242622	2.415723	0.503677	1	-0.346742	2.247847	1.055036
1	1.268465	2.178100	-2.519878	1	1.370782	2.897782	-1.669573
1	3.526241	3.754679	0.761265	1	2.736184	3.935409	2.255173
1	2.376798	-0.370988	0.718586	1	2.247582	-0.178726	1.160726
1	1.242447	-3.294169	-0.162357	1	1.842199	-3.025557	-0.529682
1	2.917806	-2.144986	3.600290	1	2.476587	-2.679244	3.684407
1	-0.770802	-0.424291	2.273310	1	-1.088373	-1.096448	1.912378
1	-4.317451	1.487692	4.093617	1	-5.428810	0.078463	3.029109
1	-4.730593	0.330820	2.819343	1	-5.187971	-1.019637	1.663910
1	-3.601134	-0.123556	4.097576	1	-4.427666	-1.358752	3.222219
1	0.280152	4.320391	2.752636	1	-1.137532	3.610960	3.559303
1	0.336820	3.260527	4.164637	1	-1.199592	2.283224	4.721314
1	1.386145	2.952736	2.764414	1	0.167369	2.430097	3.598011
1	-3.392281	3.797150	-1.691180	1	-3.676515	3.591042	-1.641448
1	-3.489088	2.917519	-0.159673	1	-3.937279	2.357819	-0.402427
1	-1.987944	3.735195	-0.613706	1	-2.568026	3.469943	-0.266984
1	-3.316977	0.274283	-2.824118	1	-2.674438	0.517571	-3.422527
1	-4.203750	0.823756	-1.388055	1	-3.934756	0.555322	-2.173010
1	-4.226888	1.796374	-2.866519	1	-3.829999	1.860716	-3.361809
1	-2.184954	3.047463	-3.592303	1	-1.970597	3.524837	-3.265034
1	-0.720445	3.036963	-2.599191	1	-0.770347	3.469143	-1.966544
1	-1.166948	1.605671	-3.562380	1	-0.718841	2.281980	-3.294365
1	2.405780	5.275301	-0.867648	1	1.516654	5.627513	0.691840
1	3.316655	4.607706	-2.222514	1	2.991279	5.455200	-0.257781

1	1.553105	4.606142	-2.267365	1	1.420628	5.207695	-1.024518
1	4.774588	1.044864	1.998556	1	4.103565	1.129813	3.176082
1	3.883499	2.374237	2.739947	1	2.947806	2.216032	3.948436
1	3.241252	0.719525	2.800976	1	2.493785	0.539661	3.579904
1	1.230900	0.035706	-4.274492	1	1.957070	1.224274	-3.815221
1	2.759387	0.663357	-3.605312	1	3.202150	1.908711	-2.737618
1	2.757023	-0.820171	-4.568174	1	3.644283	0.694794	-3.943215
1	3.898504	-2.023923	-2.649725	1	4.655102	-0.724648	-2.113865
1	3.885065	-0.536034	-1.691615	1	4.205605	0.484693	-0.903696
1	3.178828	-2.019230	-1.028919	1	3.694465	-1.199535	-0.700445
1	1.954340	-2.985412	-3.575761	1	3.122371	-1.717915	-3.592486
1	0.969451	-2.971454	-2.109267	1	1.936800	-2.208831	-2.378228
1	0.374749	-2.190364	-3.578373	1	1.436448	-1.211826	-3.751047
1	4.280799	-3.157226	1.210030	1	4.455336	-2.989158	1.722189
1	3.600065	-4.336769	2.329867	1	3.661646	-4.526662	2.055309
1	3.189364	-4.409697	0.609994	1	3.805391	-3.951977	0.389988
1	0.018836	-0.486936	4.815199	1	-0.675436	-2.041126	4.635024
1	1.769170	-0.642153	5.040266	1	0.944362	-1.478350	5.057531
1	1.096550	0.701150	4.099920	1	-0.215510	-0.379441	4.283704
1	-4.049567	-3.236810	-0.195583	1	-3.266963	-3.630974	-1.774324
1	-3.711304	-1.642727	0.478398	1	-3.341335	-2.227352	-0.707710
1	-3.391785	-1.969179	-1.239254	1	-2.678344	-2.064349	-2.347975
1	-2.830645	-4.094713	1.681849	1	-2.253289	-4.794126	0.035252
1	-1.109758	-3.783851	1.958762	1	-0.704816	-4.343100	0.762293
1	-2.299792	-2.511378	2.274797	1	-2.153078	-3.380679	1.097581
1	-1.472199	-3.760959	-1.770921	1	-0.388445	-3.368642	-2.846482
1	-0.595324	-4.471941	-0.395399	1	0.339683	-4.301734	-1.517975
1	-2.299895	-4.855002	-0.643856	1	-1.196984	-4.815672	-2.214231
23	-0.703494	-0.545339	-1.434445	23	-0.298990	-0.266544	-1.601966
8	-1.715757	-1.617286	-2.493664	8	-0.891174	-1.161178	-3.066606
8	-1.145222	-0.503198	-3.177909	8	-0.390106	0.142363	-3.351169

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