Monodentate phosphine substitution in $[Pd(\kappa^3\text{-dppf})(PR_3)][BF_4]_2$ (dppf = 1,1′-bis(diphenylphosphino)ferrocene) compounds

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Supporting Information

Stopped-flow kinetics

I. Initial results

To determine the mechanism responsible for the production of [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$, six solutions of P(*p*-$C_6H_4OCH_3)_3$ in acetone were prepared. The concentrations were 0.245 mM, 0.490 mM, 0.98 mM, 1.47 mM, 1.96 mM, and 2.45 mM. To record the reactions, 0.1 mL of each phosphine solution was mixed with 0.1 mL of 0.490 mM [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$. The kinetic traces were recorded at 364 nm. Although the signal is dominated by the production of [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$, there is an offset due to a smaller absorption signal obtained for P(*p*-$C_6H_4OCH_3)_3$ alone. The kinetics signals used for each trace were averaged over ten traces. The individual scans, along with the average signal, are shown in Fig. S1. Ten traces were measured for each concentration of P(*p*-$C_6H_4OCH_3)_3$ employed in this study. The averaged scans for the six reactions measured in this work are shown in Fig. S2. For comparative purposes, each scan was normalized for fitting analysis in Sections II and III.

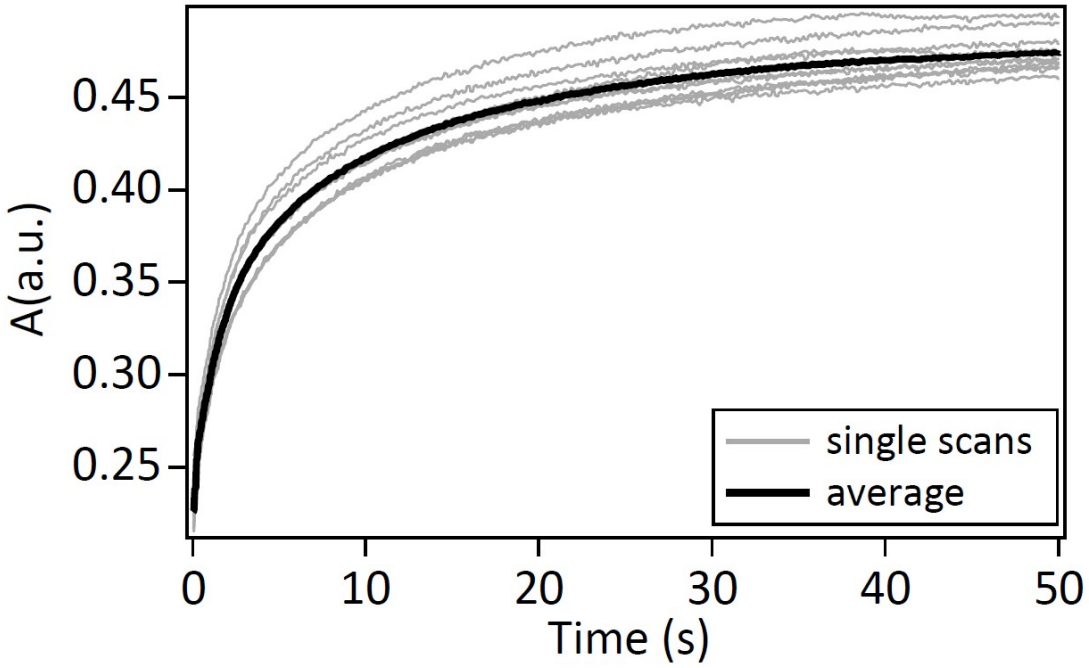


Fig. S1 Kinetic traces of the formation of [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$ using the mixture of 0.49 mM [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ and 2.45 mM P(*p*-$C_6H_4OCH_3)_3$. Ten scans were recorded. The average of the scans, which is shown in black, was used for fitting analysis.

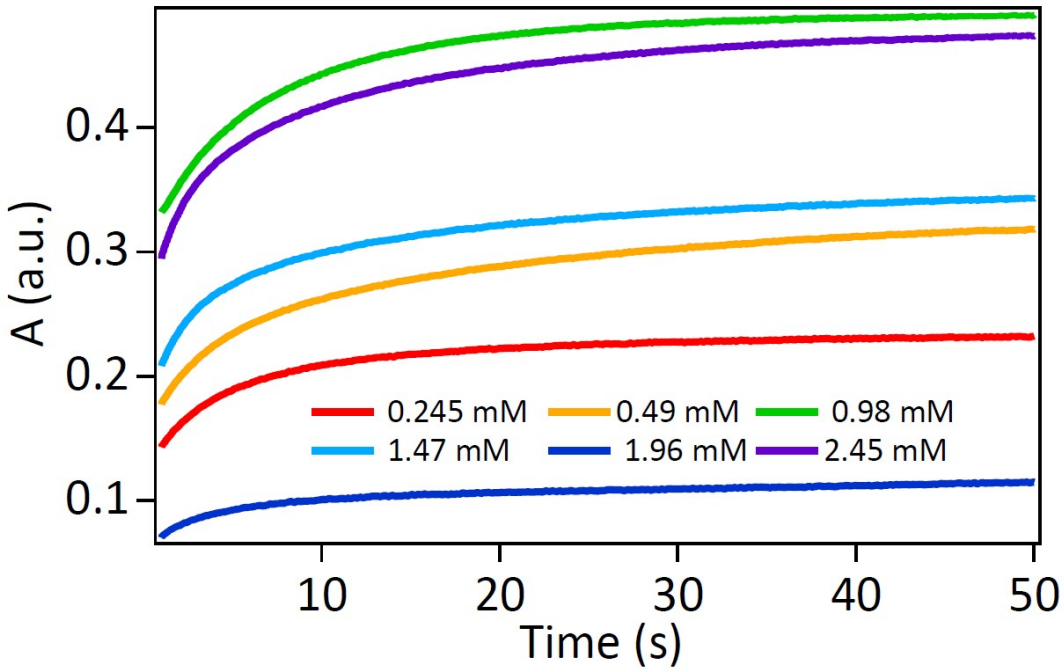


Fig. S2 Averaged signal for the six reactions of [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ with P(*p*-$C_6H_4OCH_3)_3$. For each trace, [P(*p*-$C_6H_4OCH_3)_3$] is indicated.

All fits were performed using IgorPro software. When differential equations were used, the fits were compared to models in Mathematica to verify the consistency of these fits. Initially, the scans were fit to a single exponential decay. The assumption was that there was a rate-determining step that would dominate the process of the formation of [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$. This fit is shown in Fig. S3. The first 350 ms were not used in the fit because mixing effects were observed in the first few hundred ms of all traces. The fits shown in Fig. S3 do not show reasonable agreement with the experimental traces. Therefore, a double exponential model was used initially to fit this trace. The result of this fit is shown in Fig S4. The result of this double exponential fit is reasonable, but it does not accurately portray an effective dissociative mechanism for this chemical reaction. To accurately portray the model for the formation of [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$, the following procedures were used: 1) the double exponential fits were used to qualitatively assess the dependence of the concentration of P(*p*-$C_6H_4OCH_3)_3$ on the rate of reaction; 2) a purely associative model was ruled out; and 3) a dissociative model is proposed and determined to be the best model to explain the rate dependencies of this reaction.

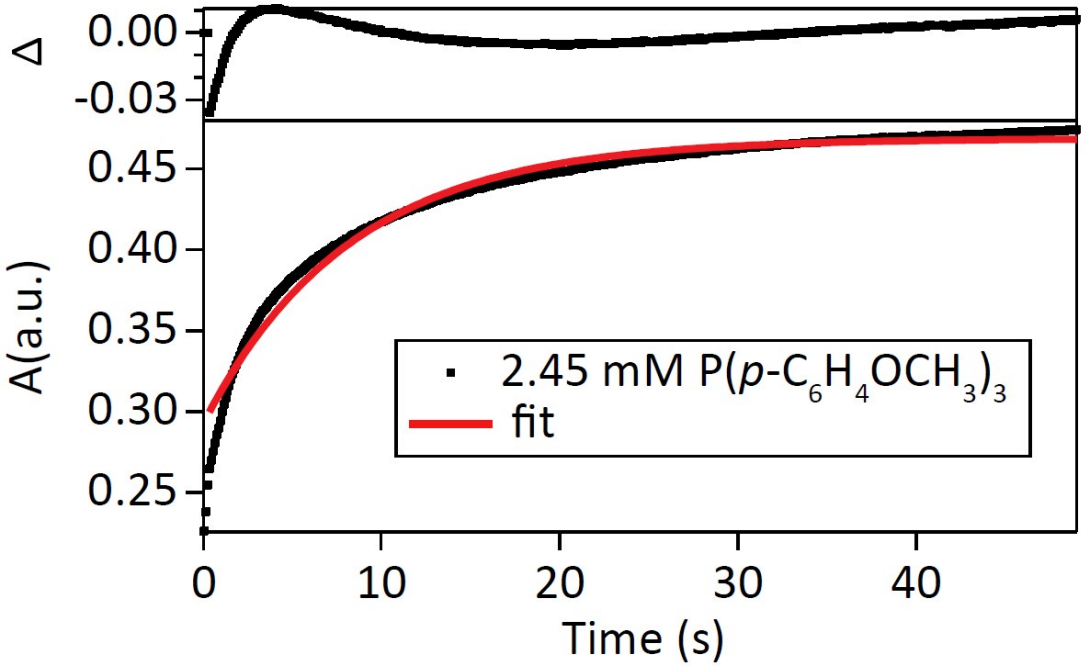


Fig. S3 The averaged kinetics trace shown in Fig. S1 fit to a single exponential. The concentration of the P(*p*-$C_6H_4OCH_3)_3$ ligand was 2.45 mM.

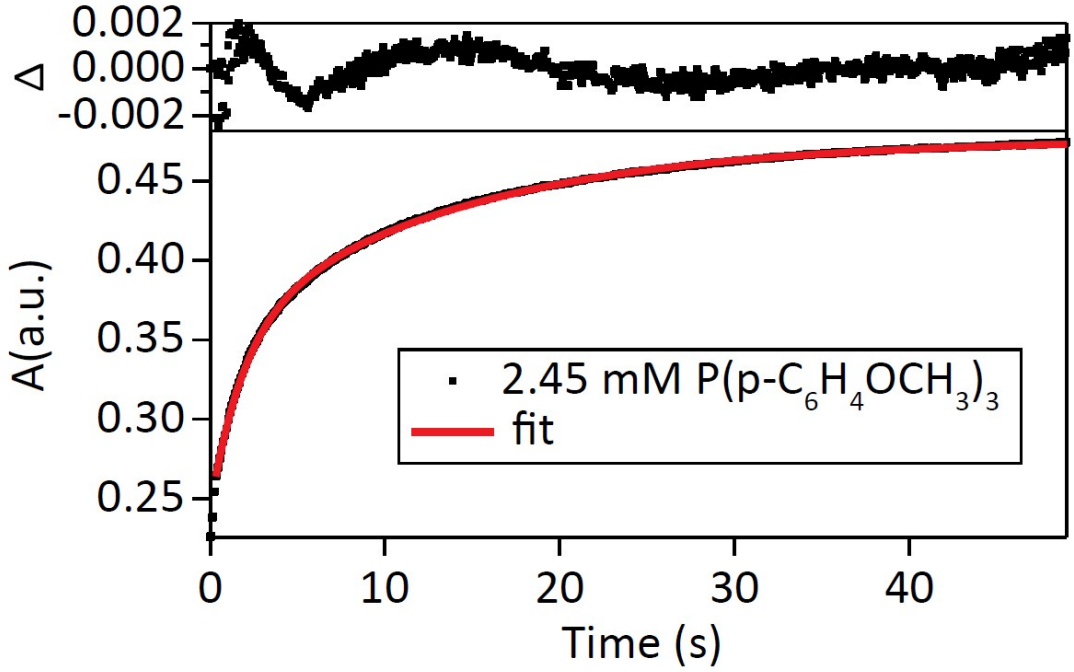


Fig. S4 The averaged kinetics trace shown in Fig. S1 and S3 fit to a double exponential.

II. Double exponential fitting

The time constants for the double exponential fits is shown in Table S1. The fits do not show a large difference in the time constants or amplitudes. The second time constant of entry

5 is in bold because it is an outlier. Therefore, this trace was not used for further analysis. The dependence of the rates on the incoming ligand is also shown in Fig. S5. A slight negative dependence on the time constant was recorded for these data sets. Therefore, the mechanism of [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$ formation is not largely dependent on the concentration of the incoming ligand, but a slight dependence is observed. Therefore, the reaction mechanism was considered in more detail to better determine the pathways used in formation of this complex.

Table S1 Individual fitting results using a double exponential model.

entry	[P(*p*-$C_6H_4OCH_3)_3$]	A1	τ 1	A2	τ 2
1	0.245	-0.0509131	3.17203	-0.0397157	14.648
2	0.490	-0.0555357	3.04788	-0.0959159	21.7039
3	0.980	-0.0609013	3.51219	-0.101745	10.6368
4	1.47	-0.0598301	2.22538	-0.0798075	16.9355
5	1.96	-0.0275625	3.36158	-0.0292193	**64.681**
6	2.45	-0.0693585	2.03445	-0.113464	13.9116

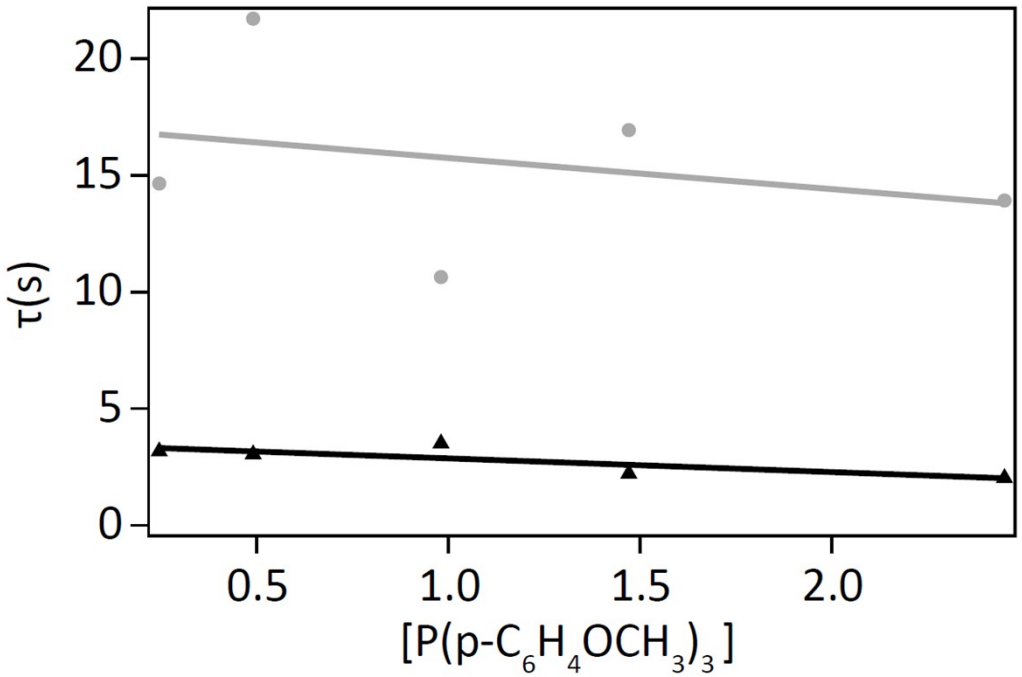
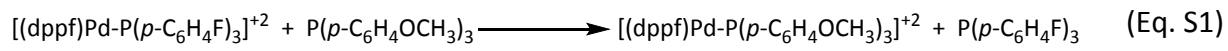


Fig. S5 Time constant fits for entries 1-4 and 6 recorded in Table S1.

III. Associative mechanism

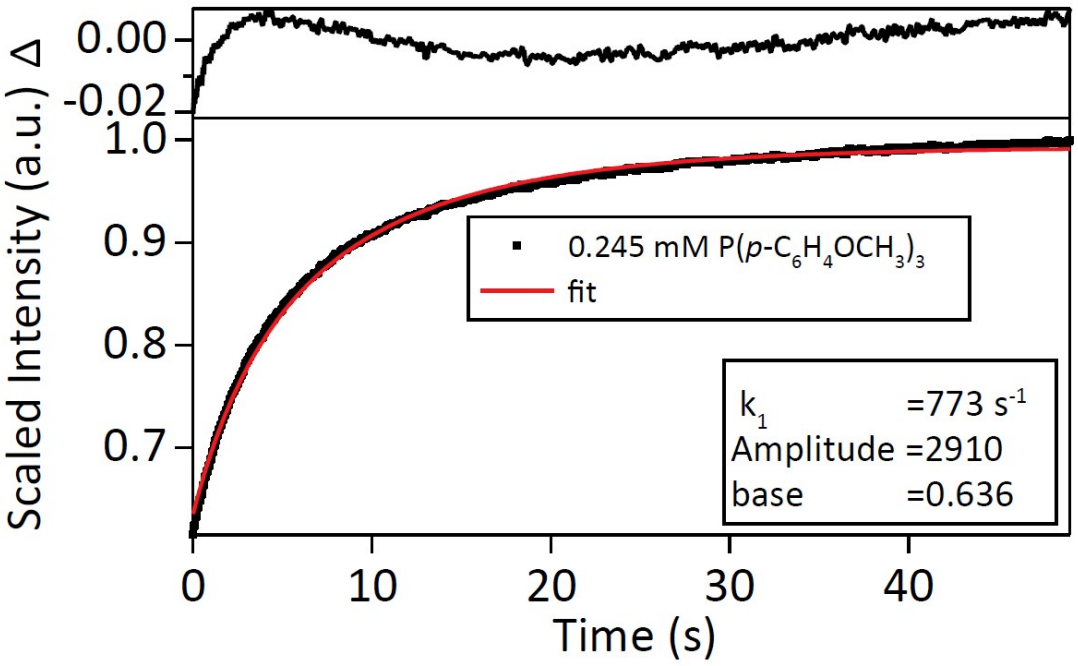
There are two general mechanisms that are possible for ligand substitution: associative and dissociative. To rule out the associative pathways, we used the following mechanism (Eq. S1) to fit the results. The concentrations of both reactants was comparable, so the pseudo-first



(Eq. S1)

order approximation was not used. The individual fits using this model are reasonable, but the time constants vary widely. Two examples of fits using this model are shown in Fig. S6. The disagreement of the rate constants obtained in these fits verifies that another reaction mechanism is necessary for the [Pd(dppf)(P(*p*-$C_6H_4OCH_3$)$_3$)][BF_4]$_2$ formation. The residuals are not reasonable for all traces, and the rate constant decreases with increasing (P(*p*-$C_6H_4OCH_3$)$_3$ concentration.

(a)



(b)

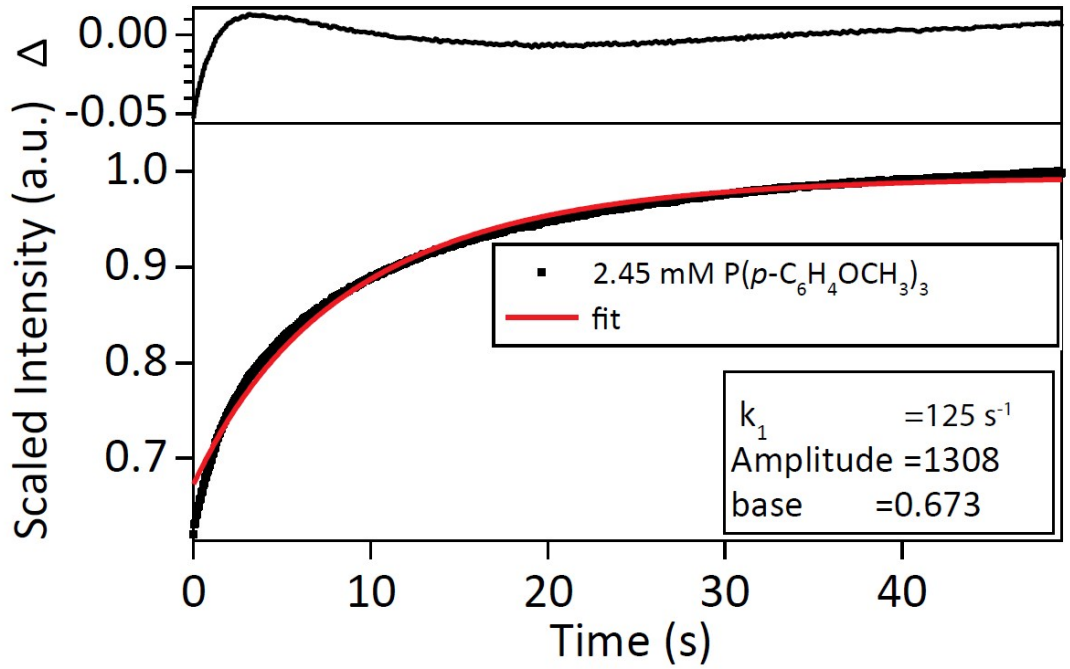
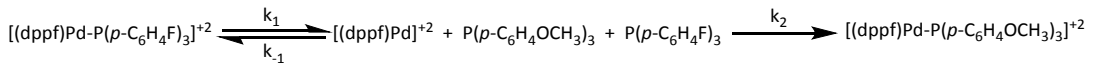


Fig. S6. Associative mechanism fits using a) 0.245 mM P(*p*-$C_6H_4OCH_3$)$_3$ and b) 2.45 mM P(*p*-$C_6H_4OCH_3$)$_3$. The time constants and amplitudes for these fits are shown in the insets.

IV. Dissociative mechanism

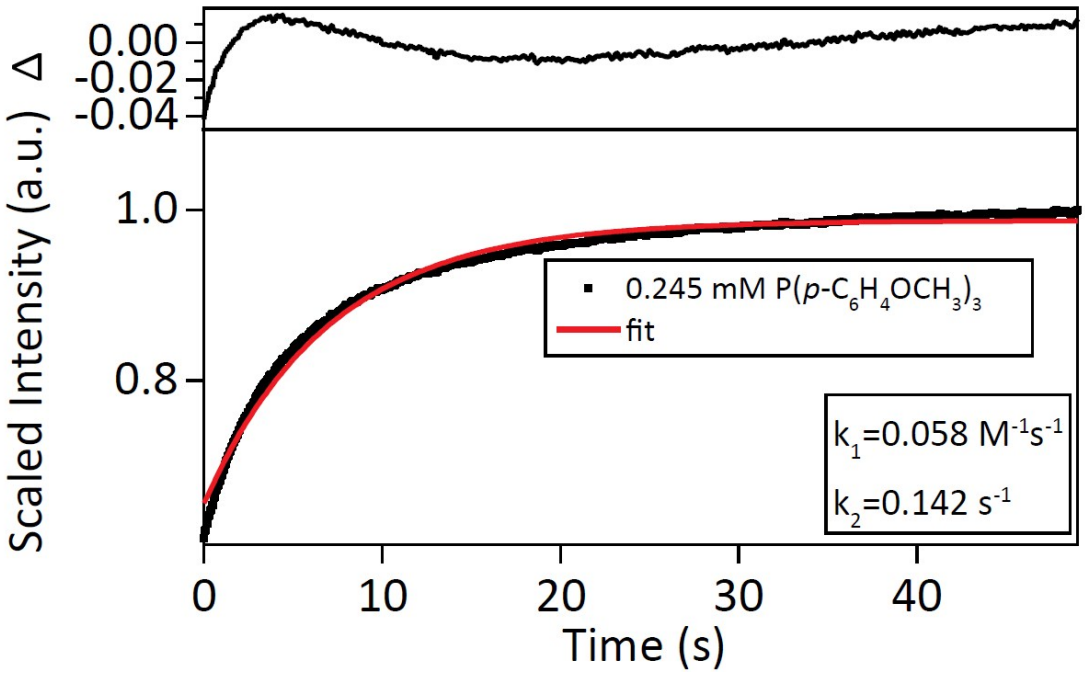
The following dissociative reaction mechanism was proposed for [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$ formation (Eq. S2). The mechanism assumes that $k_1 << k_{-1}$. The dissociation of



(Eq. S2)

[Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ is not observed in solution. The NMR results of the neat solution did not indicate the presence of free ligand or the unligated complex, $[Pd(dppf)]^{+2}$. Therefore, it is assumed that $K_{eq} << 1$. This mechanism was also used to verify this claim. Initially, each trace was fit using this mechanism. The combined associative/dissociative mechanism fits are shown below in Fig. S7. The proposed reaction mechanism for these fits is shown in Eq. S3. The fits for the dissociative mechanism (Eq. S2) are shown in Fig. S8. Compared to the combined associative/dissociative mechanism, these fits are much more reliable. Therefore, we have verified that the dissociation mechanism is the preferred formation mechanism for this ligand exchange.

(a)



(b)

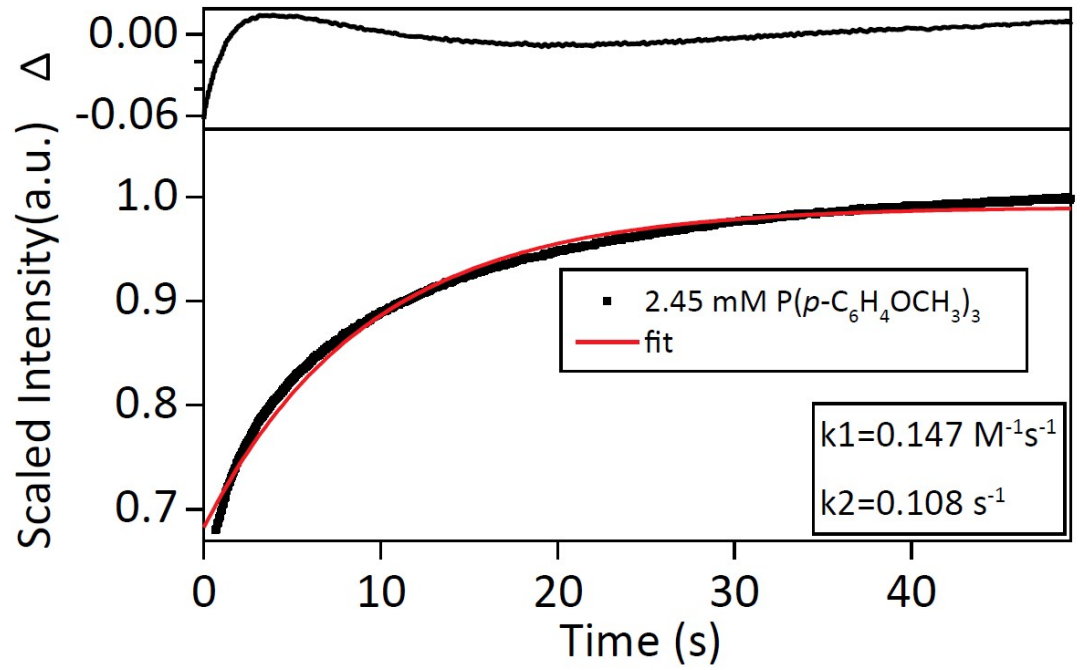
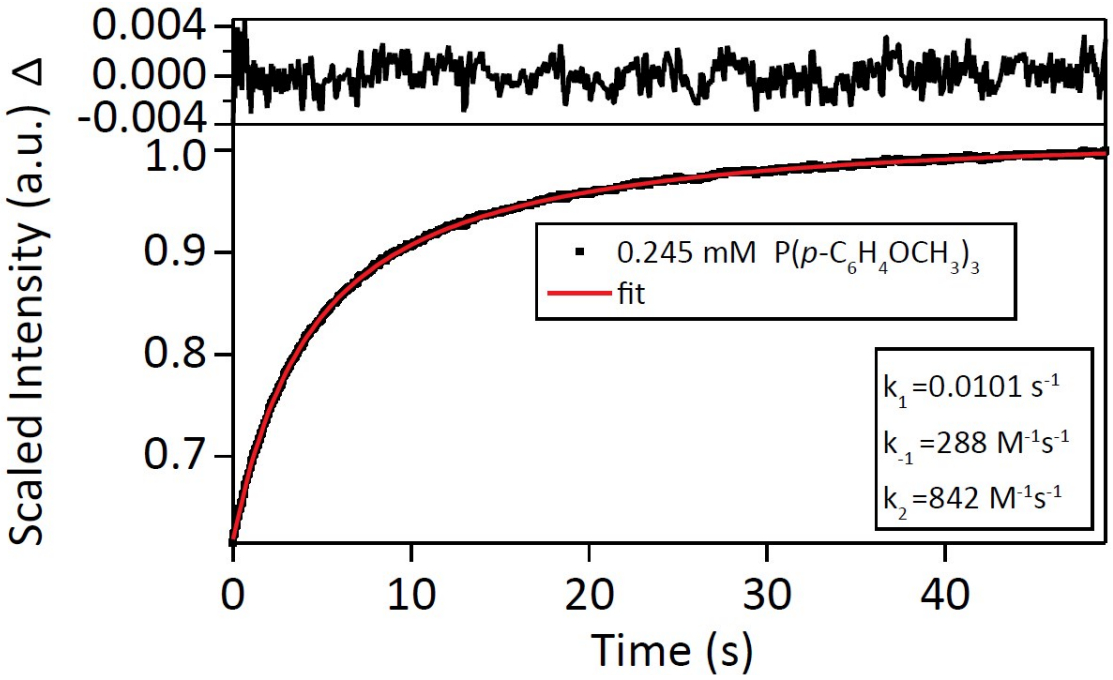


Fig. S7 Combined associative/dissociative mechanism fits using a) 0.245 mM P(*p*-$C_6H_4OCH_3$)$_3$ and b) 2.45 mM P(*p*-$C_6H_4OCH_3$)$_3$. The time constants for these fits are shown in the insets.

1) $[(dppf)Pd\text{-}P(p\text{-}C_6H_4F)_3]^{+2} + P(p\text{-}C_6H_4OCH_3)_3 \xrightarrow{k_1} [(dppf)Pd\text{-}P(p\text{-}C_6H_4OCH_3)_3]^{+2} + P(p\text{-}C_6H_4F)_3$

2) $[(dppf)Pd\text{-}P(p\text{-}C_6H_4F)_3]^{+2} \xrightarrow[P(p\text{-}C_6H_4OCH_3)_3]{k_2} [(dppf)Pd\text{-}P(p\text{-}C_6H_4OCH_3)_3]^{+2} + P(p\text{-}C_6H_4F)_3$ (Eq. S3)

(a)



(b)

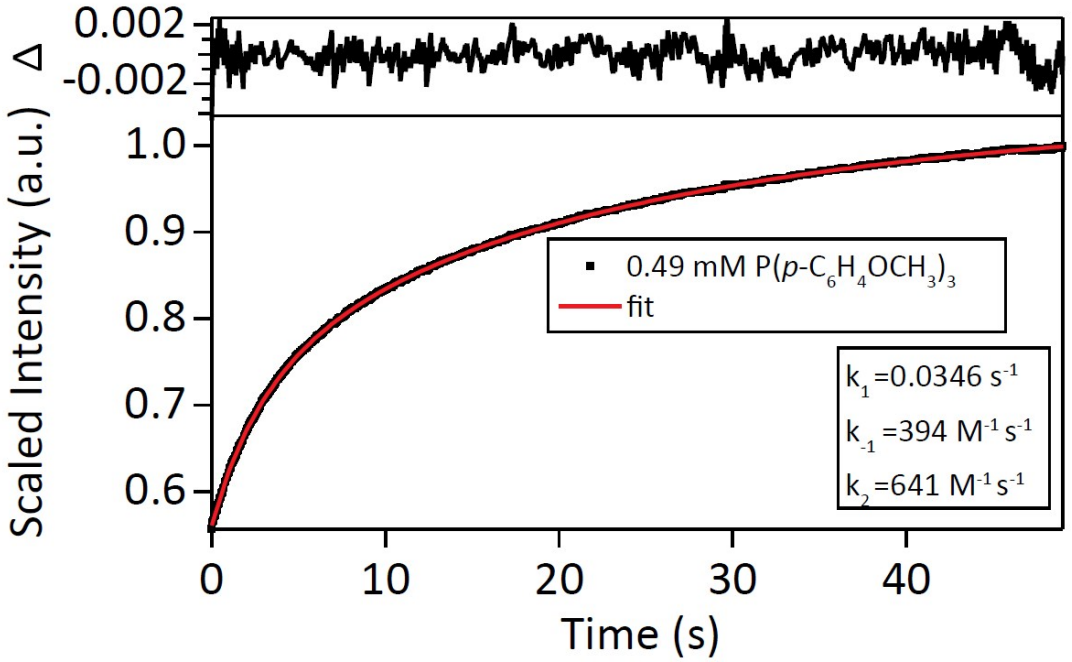


Fig. S8 The three component dissociative mechanism fits using a) 0.245 mM P(p-$C_6H_4OCH_3$)$_3$ and b) 0.45 mM P(p-$C_6H_4OCH_3$)$_3$. The time constants for these fits are shown in the insets.

Finally, the kinetic traces of the average scans of the [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ + P(*p*-$C_6H_4OCH_3)_3$ reaction using P(*p*-$C_6H_4OCH_3)_3$ concentrations of 0.245 mM, 0.49 mM, 0.98 mM, 1.47 mM, and 2.45 mM were fit using a global, genetic fitting algorithm. The variation of the rate constants is minimized using this fitting method. Initially, the concentrations of all species were kept constant to get initial time constants. The concentrations were then allowed to vary by ten percent for each trace to account for the time offset due to mixing. The time constants were then fit again using global fitting analysis (Fig 3 in the paper). These fits indicate that the rate limiting step will be the dissociation of the [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ compound. The addition of either the P(*p*-$C_6H_4F)_3$ or the P(*p*-$C_6H_4OCH_3)_3$ ligand will occur at similar rates, but the addition of P(*p*-$C_6H_4OCH_3)_3$ is a little faster. The dissociation of the [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$ compound was not determined because no appreciable amount of [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ is left in solution as no NMR signal for the compound was observed.

UV-visible spectra

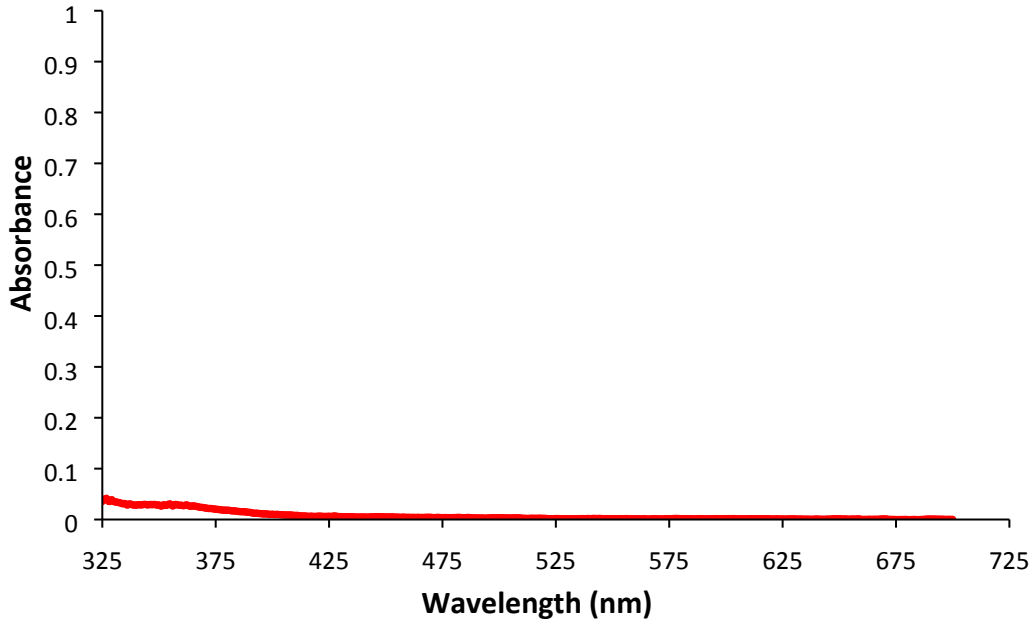


Fig. S9 UV-visible spectrum of 0.098 mM P(*p*-$C_6H_4OCH_3$)$_3$ in acetone.

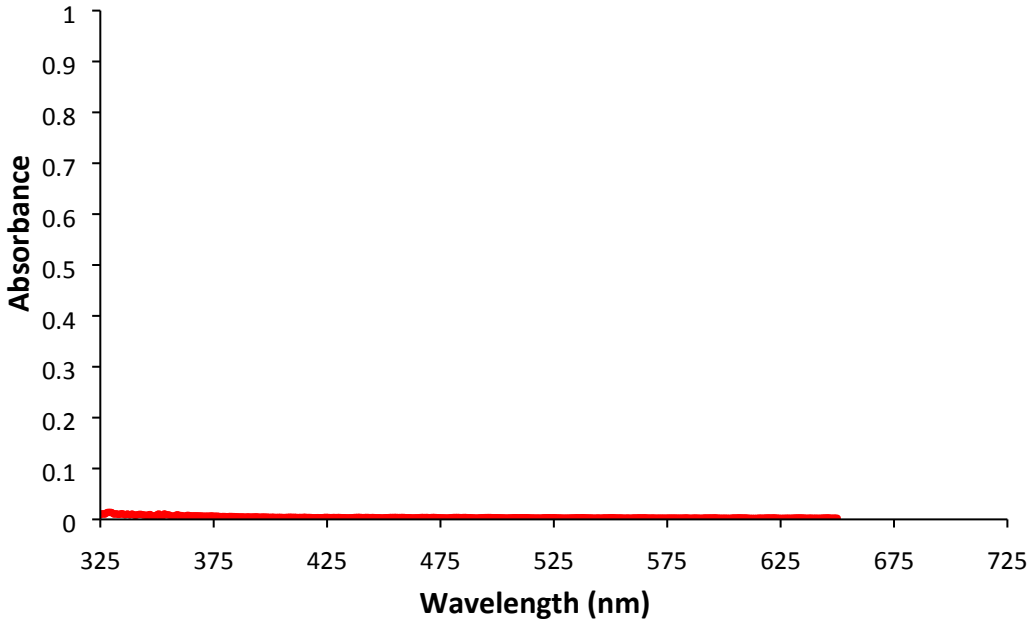


Fig. S10 UV-visible spectrum of 0.098 mM P(*p*-$C_6H_4F)_3$ in acetone.

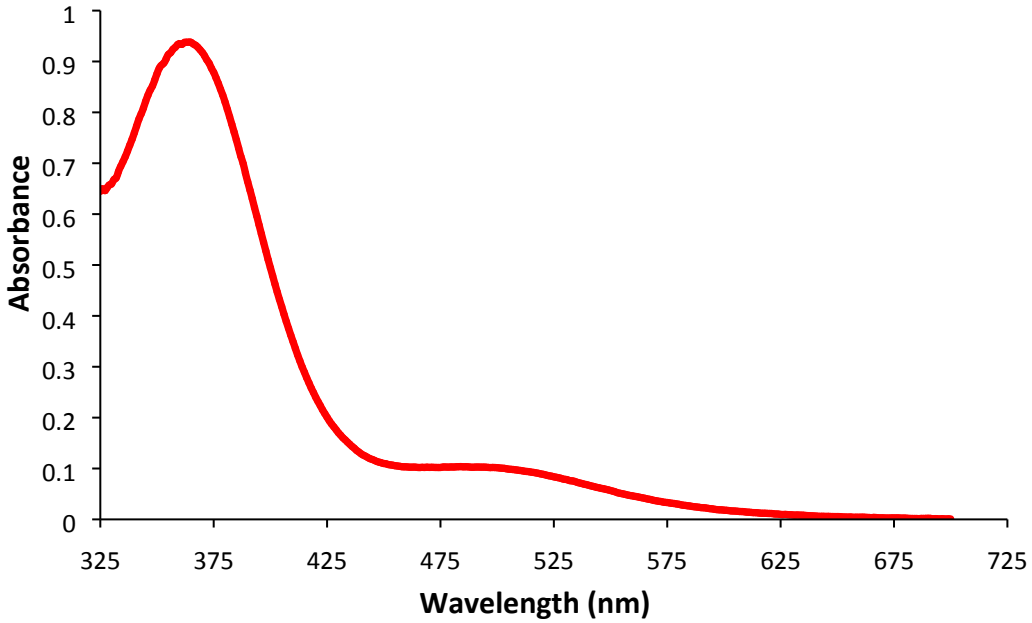


Fig. S11 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$ in acetone.

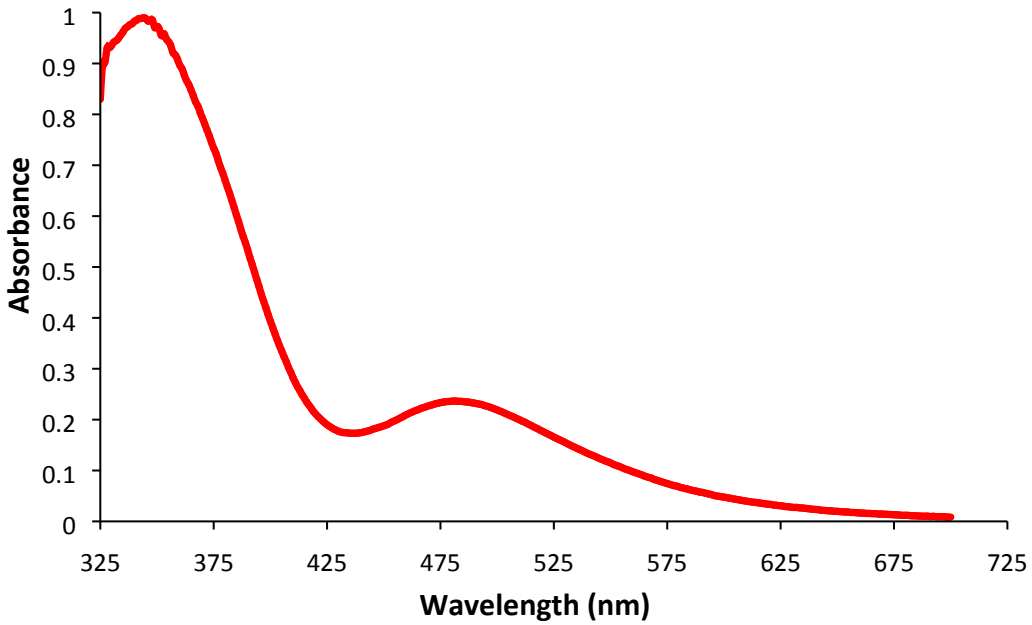


Fig. S12 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(*p*-$C_6H_4CH_3)_3$)][BF_4]$_2$ in acetone.

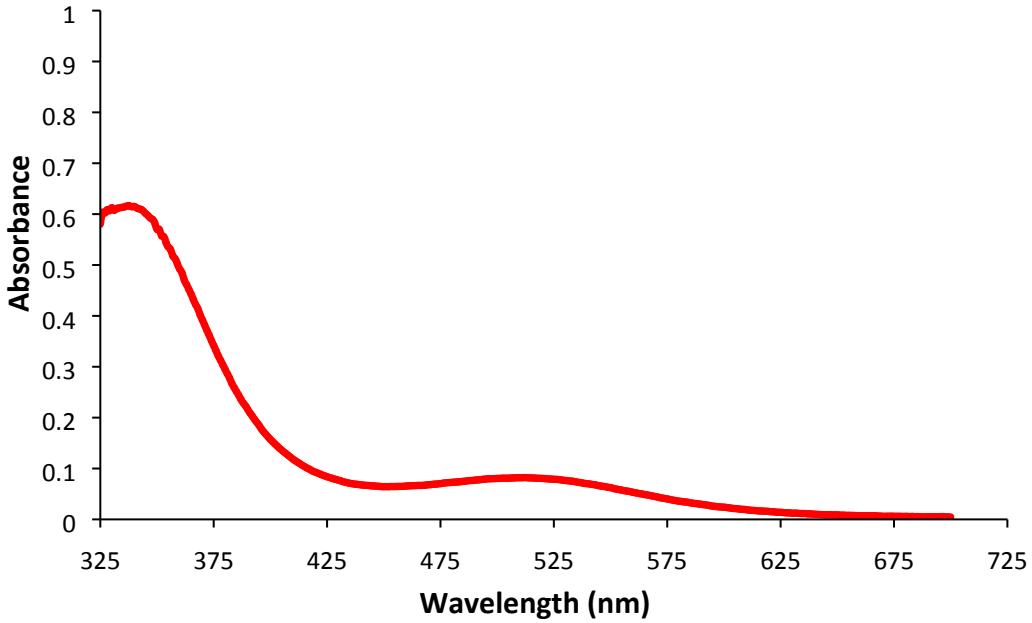


Fig. S13 UV-visible spectrum of 0.098 mM $[Pd(dppf)PPh_3][BF_4]_2$ in acetone.

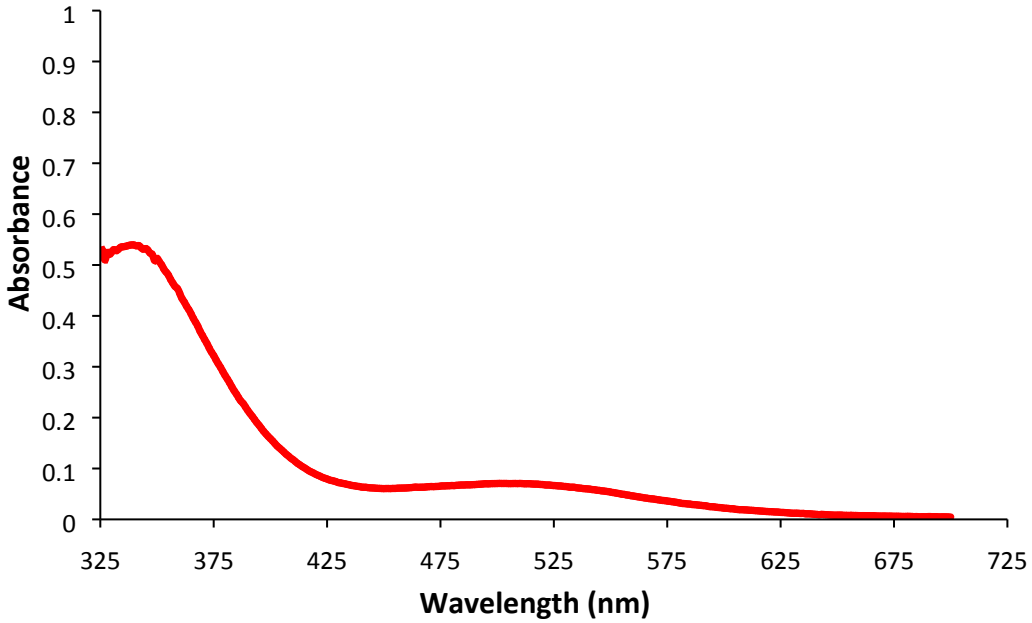


Fig. S14 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(p-$C_6H_4F)_3$)][BF_4]$_2$ in acetone.

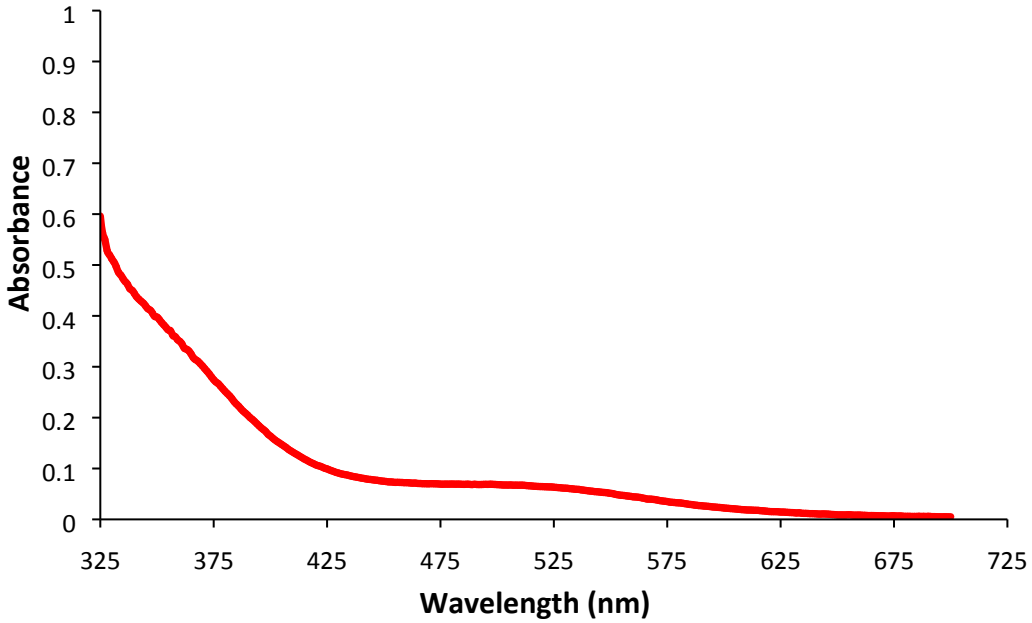


Fig. S15 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(p-$C_6H_4CF_3$)$_3$)][BF_4]$_2$ in acetone.

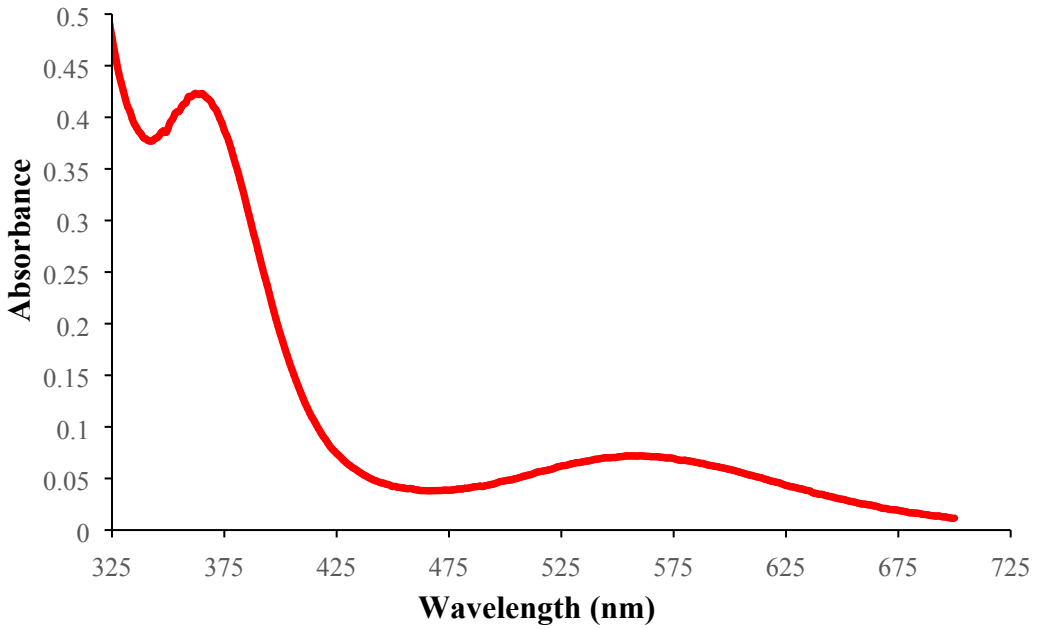


Fig. S16 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(p-$C_6H_4CF_3$)$_3$)][BF_4]$_2$ in MeCN.

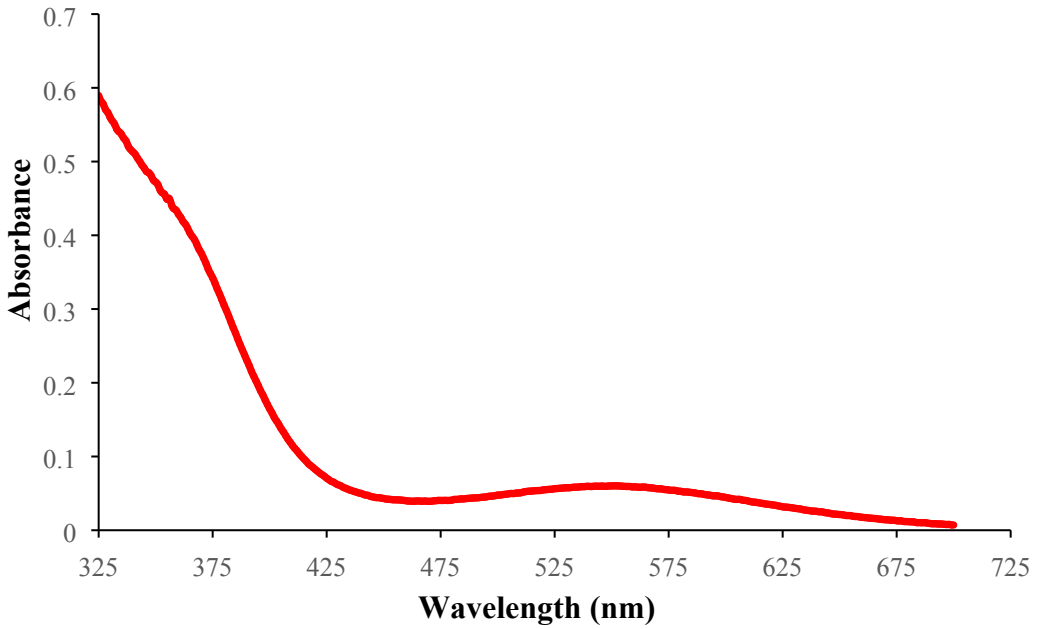


Fig. S17 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(p-$C_6H_4F)_3$)][BF_4]$_2$ in MeCN.

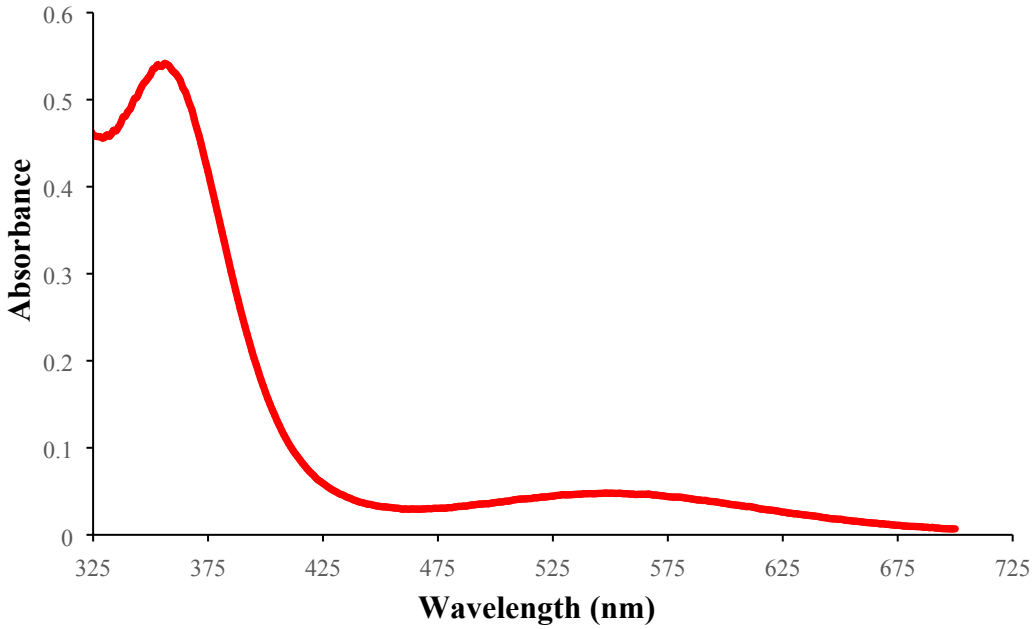


Fig. S18 UV-visible spectrum of 0.098 mM $[Pd(dppf)PPh_3][BF_4]_2$ in MeCN.

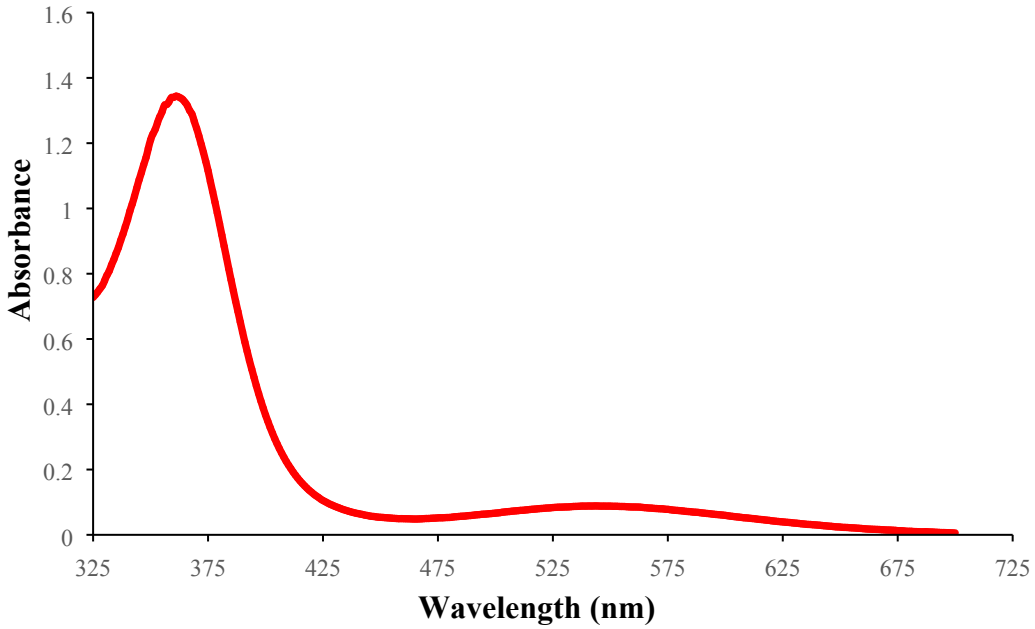


Fig. S19 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(p-$C_6H_4CH_3)_3$)][BF_4]$_2$ in MeCN.

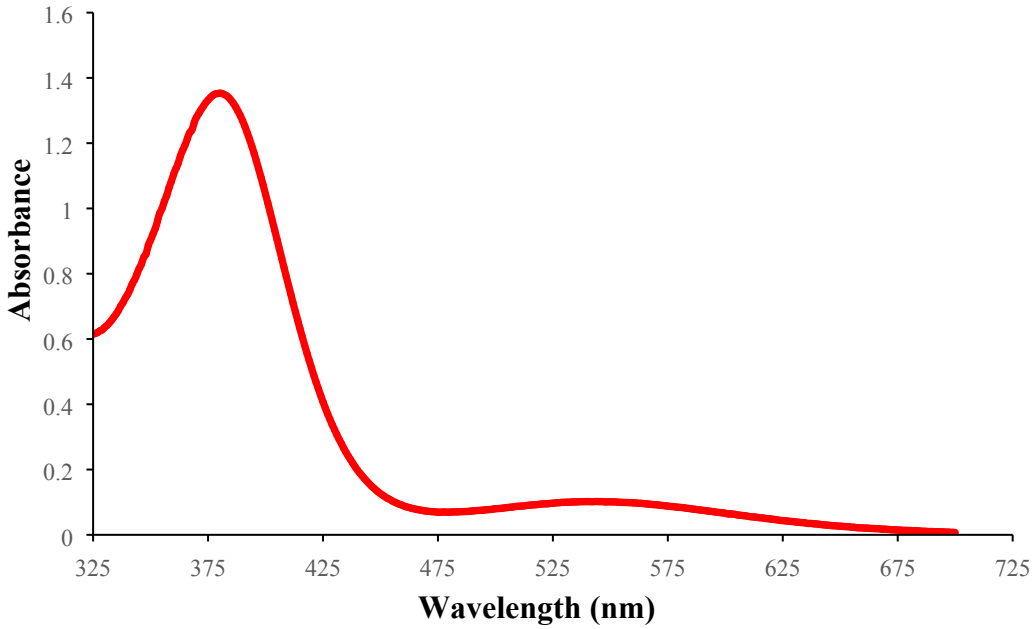


Fig. S20 UV-visible spectrum of 0.098 mM [Pd(dppf)(P(p-$C_6H_4OCH_3)_3$)][BF_4]$_2$ in MeCN.

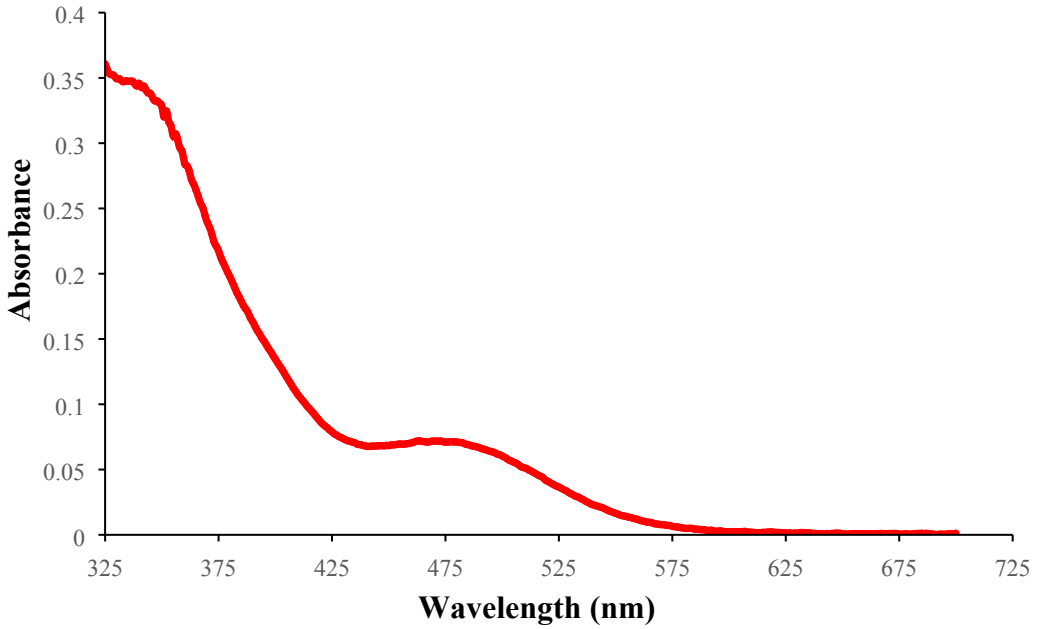


Fig. S21 UV-visible spectrum of 0.098 mM [Pd(dppf)Cl_2] in MeCN.

Cyclic voltammograms

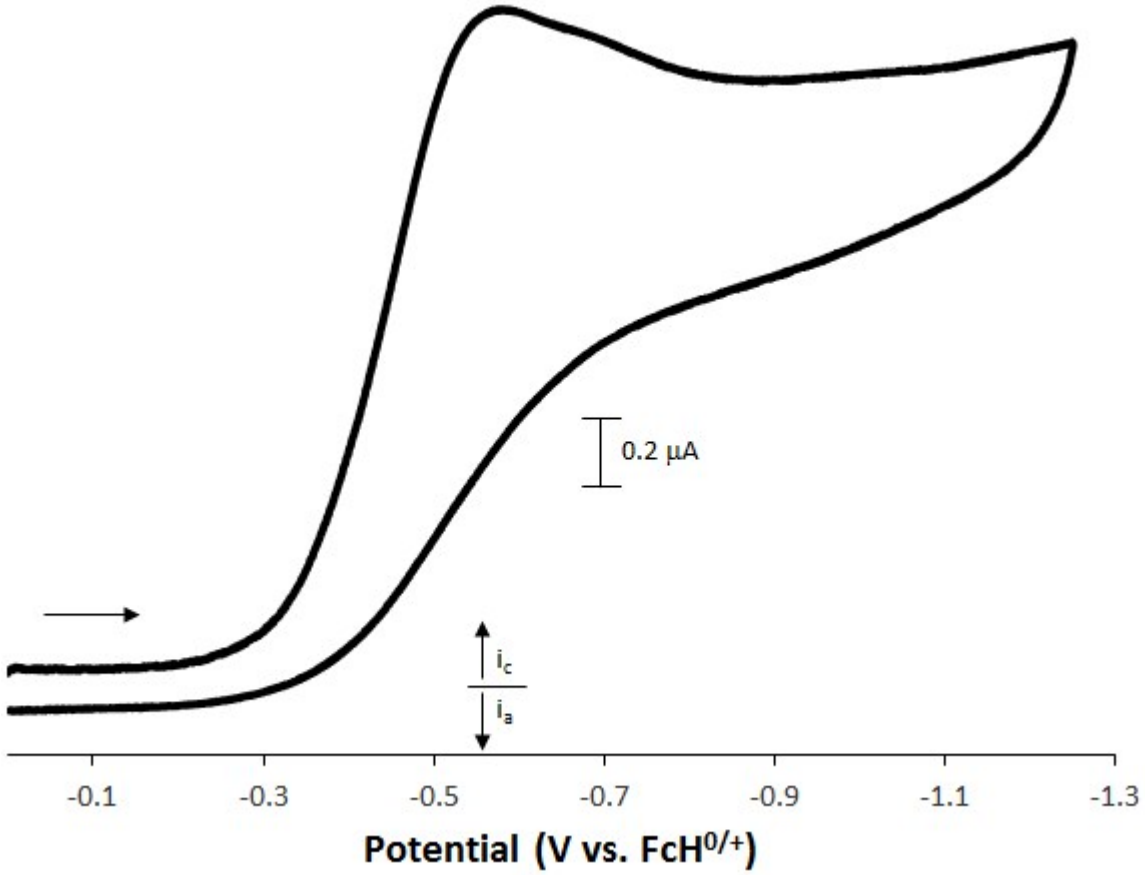


Fig. S22 CV scan for the reduction of 0.1 M [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$ in CH_2Cl_2 with [NBu_4][PF_6] as the supporting electrolyte at 100 mV s^{-1}.

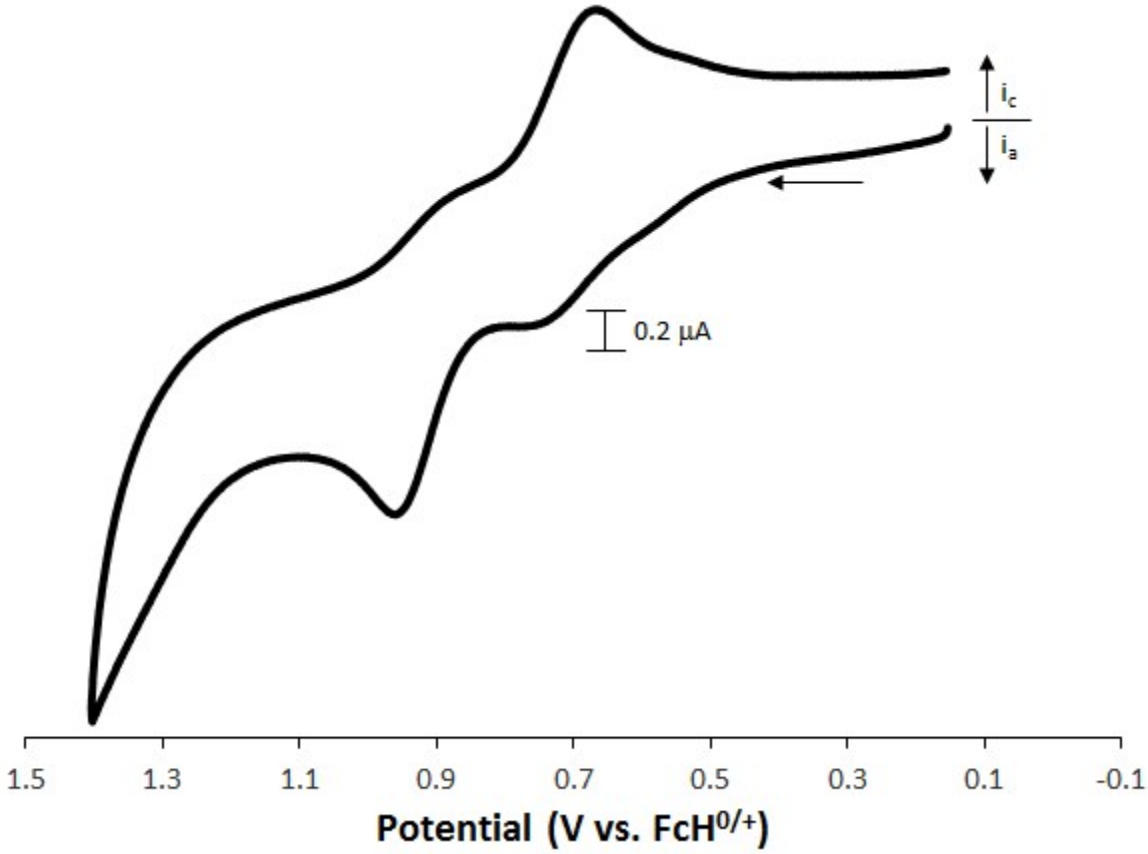


Fig. S23 CV scan for the oxidation of 0.1 M [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$ in CH_2Cl_2 with [NBu_4][PF_6] as the supporting electrolyte at 100 mV s^{-1}.

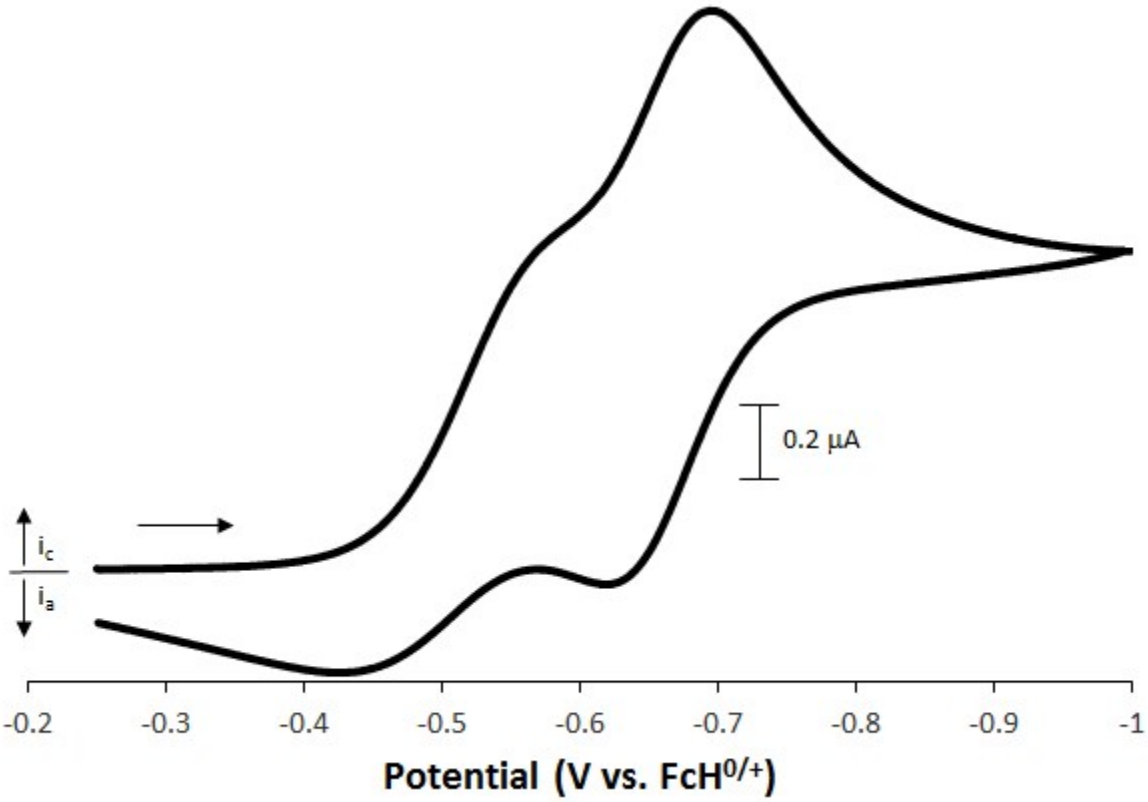


Fig. S24 CV scan for the reduction of 0.1 M $[Pd(dppf)(P(p\text{-}C_6H_4CH_3)_3)][BF_4]_2$ in CH_2Cl_2 with $[NBu_4][PF_6]$ as the supporting electrolyte at 100 mV s^{-1}.

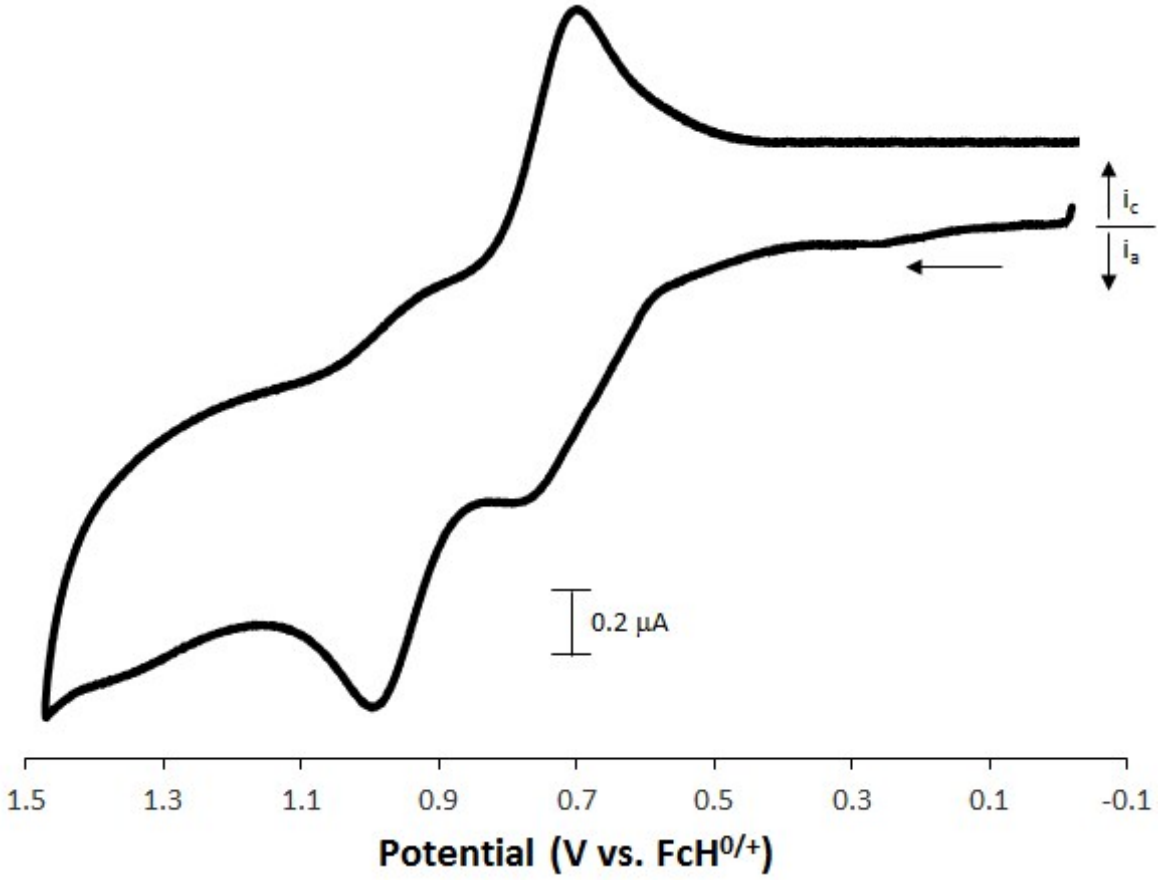


Fig. S25 CV scan for the oxidation of 0.1 M [Pd(dppf)(P(*p*-$C_6H_4CH_3)_3$)][BF_4]$_2$ in CH_2Cl_2 with [NBu_4][PF_6] as the supporting electrolyte at 100 mV s^{-1}.

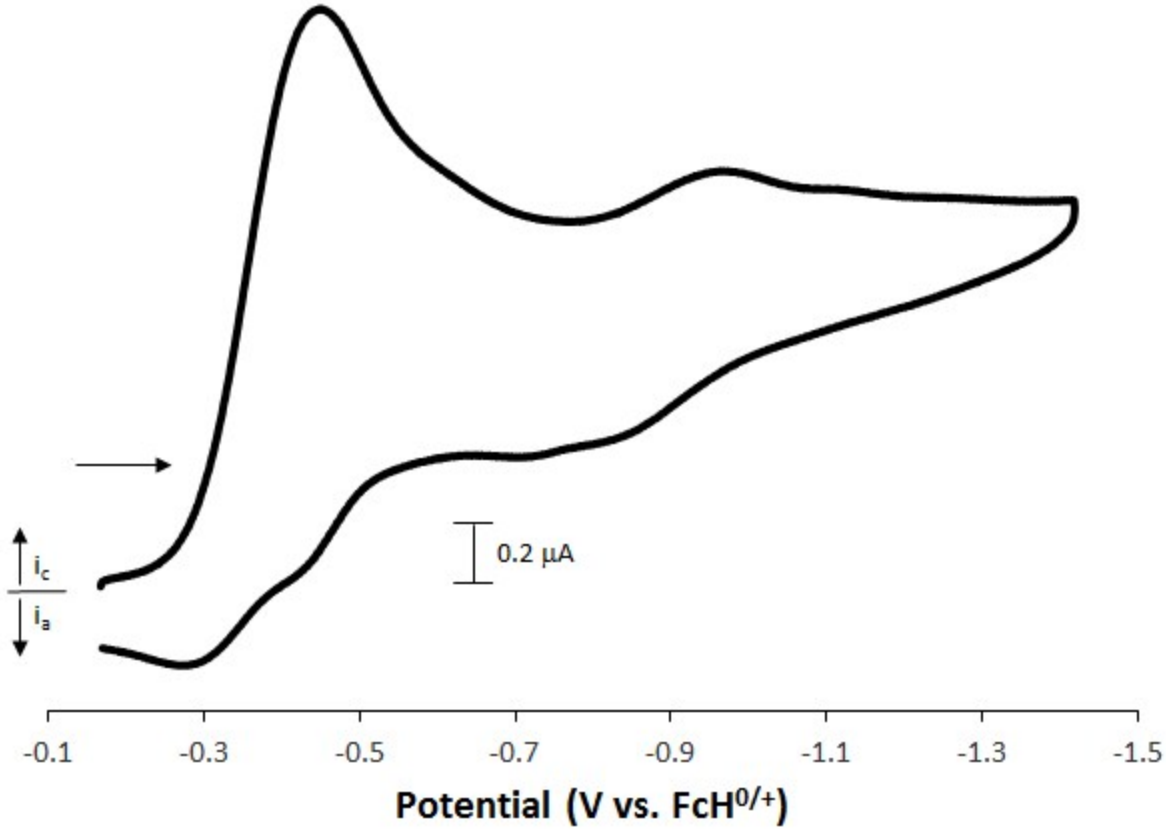


Fig. S26 CV scan for the reduction of 0.1 M [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ in CH_2Cl_2 with [NBu_4][PF_6] as the supporting electrolyte at 100 mV s^{-1}.

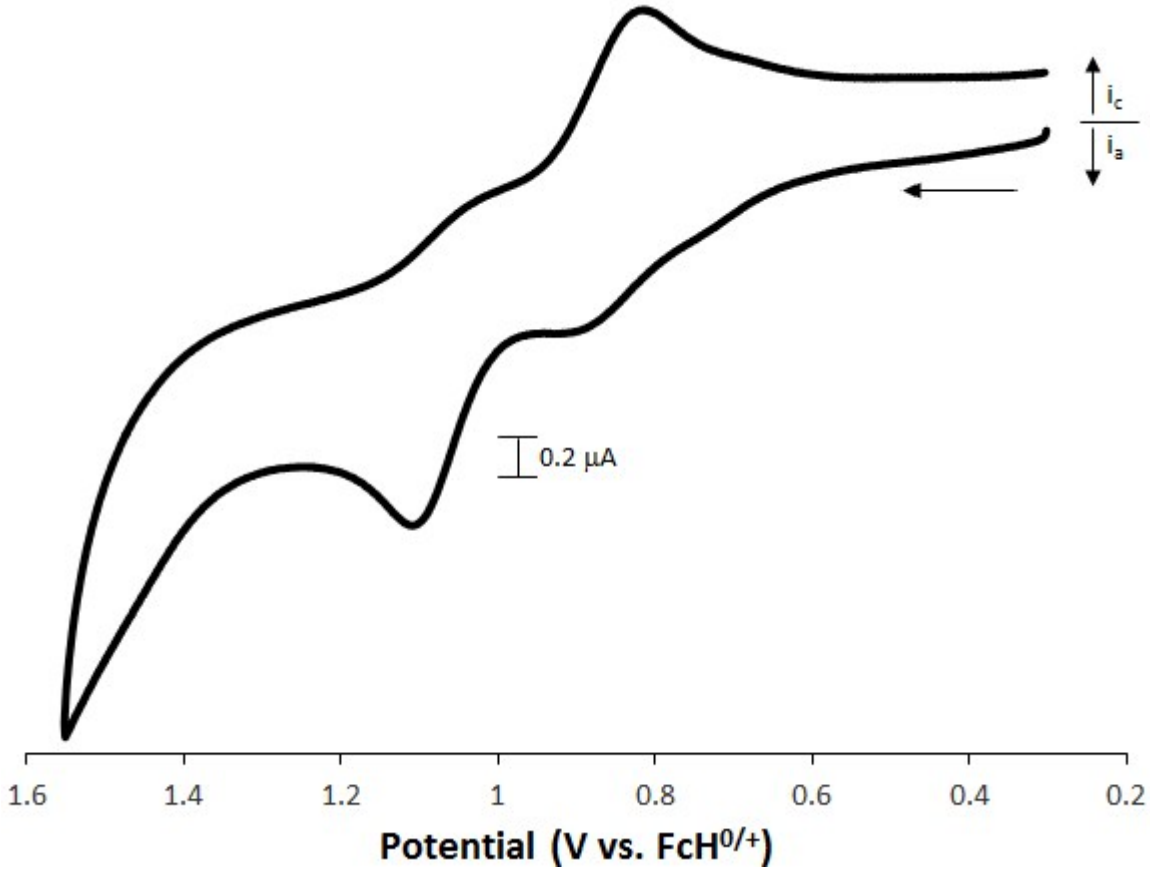


Fig. S27 CV scan for the oxidation of 0.1 M [Pd(dppf)(P(*p*-$C_6H_4F)_3$)][BF_4]$_2$ in CH_2Cl_2 with [NBu_4][PF_6] as the supporting electrolyte at 100 mV s^{-1}.

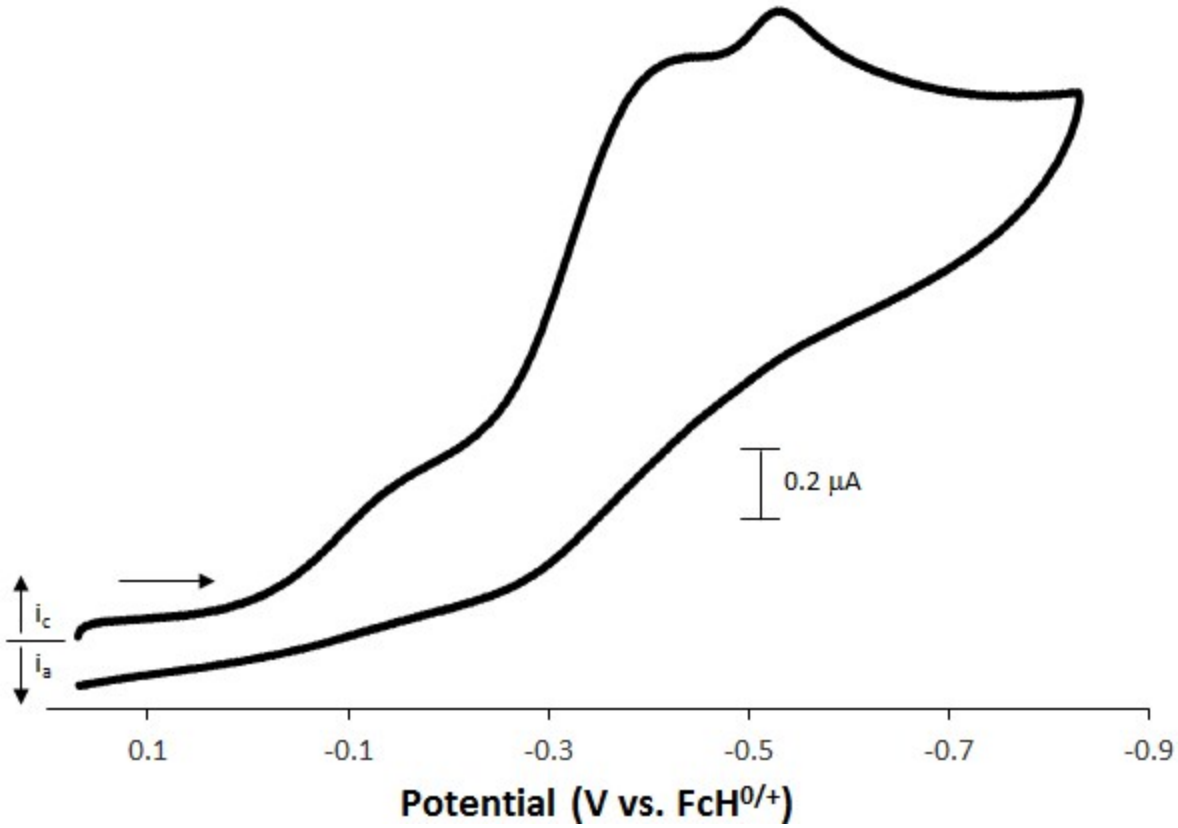


Fig. S28 CV scan for the reduction of 0.1 M [Pd(dppf)(P(*p*-$C_6H_4CF_3)_3$)][BF_4]$_2$ in CH_2Cl_2 with [NBu_4][PF_6] as the supporting electrolyte at 100 mV s^{-1}.

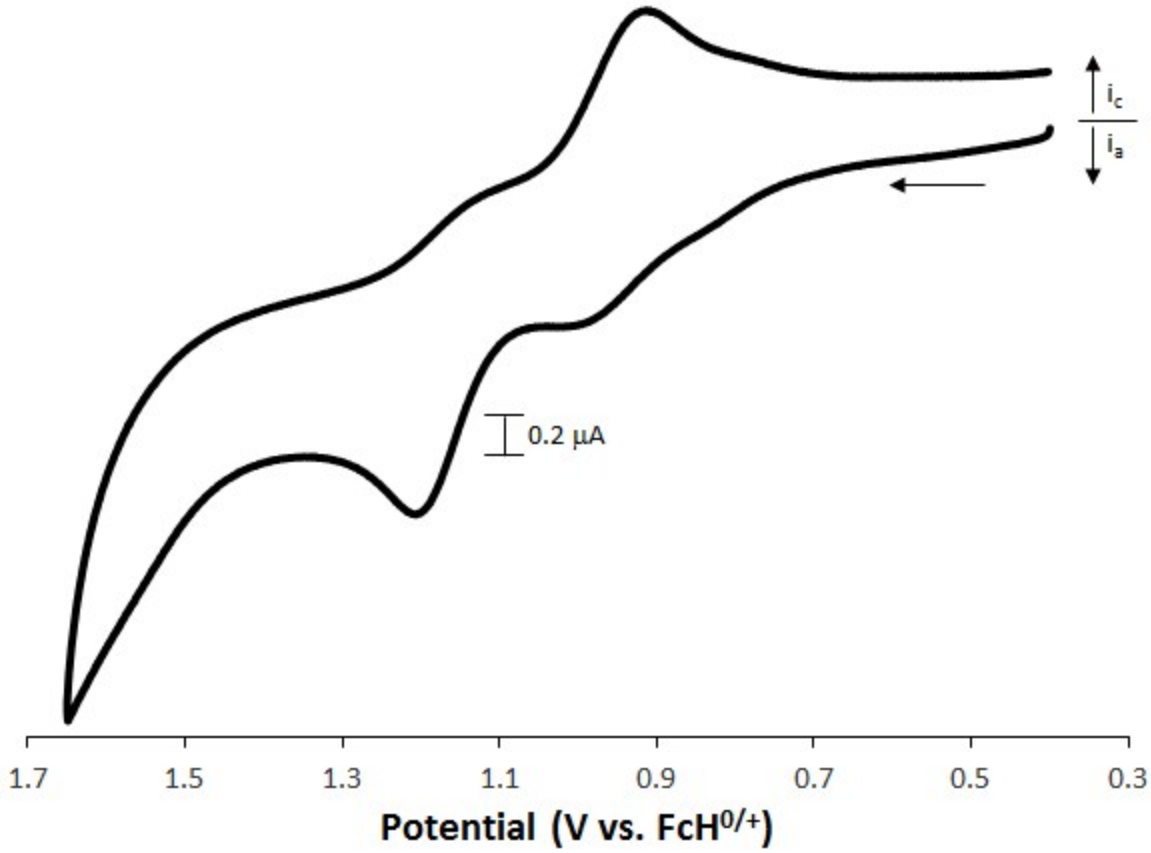


Fig. S29 CV scan for the oxidation of 0.1 M [Pd(dppf)(P(*p*-$C_6H_4CF_3)_3$)][BF_4]$_2$ in CH_2Cl_2 with [NBu_4][PF_6] as the supporting electrolyte at 100 mV s^{-1}.

$^{31}P\{^{1}H\}$ NMR spectra

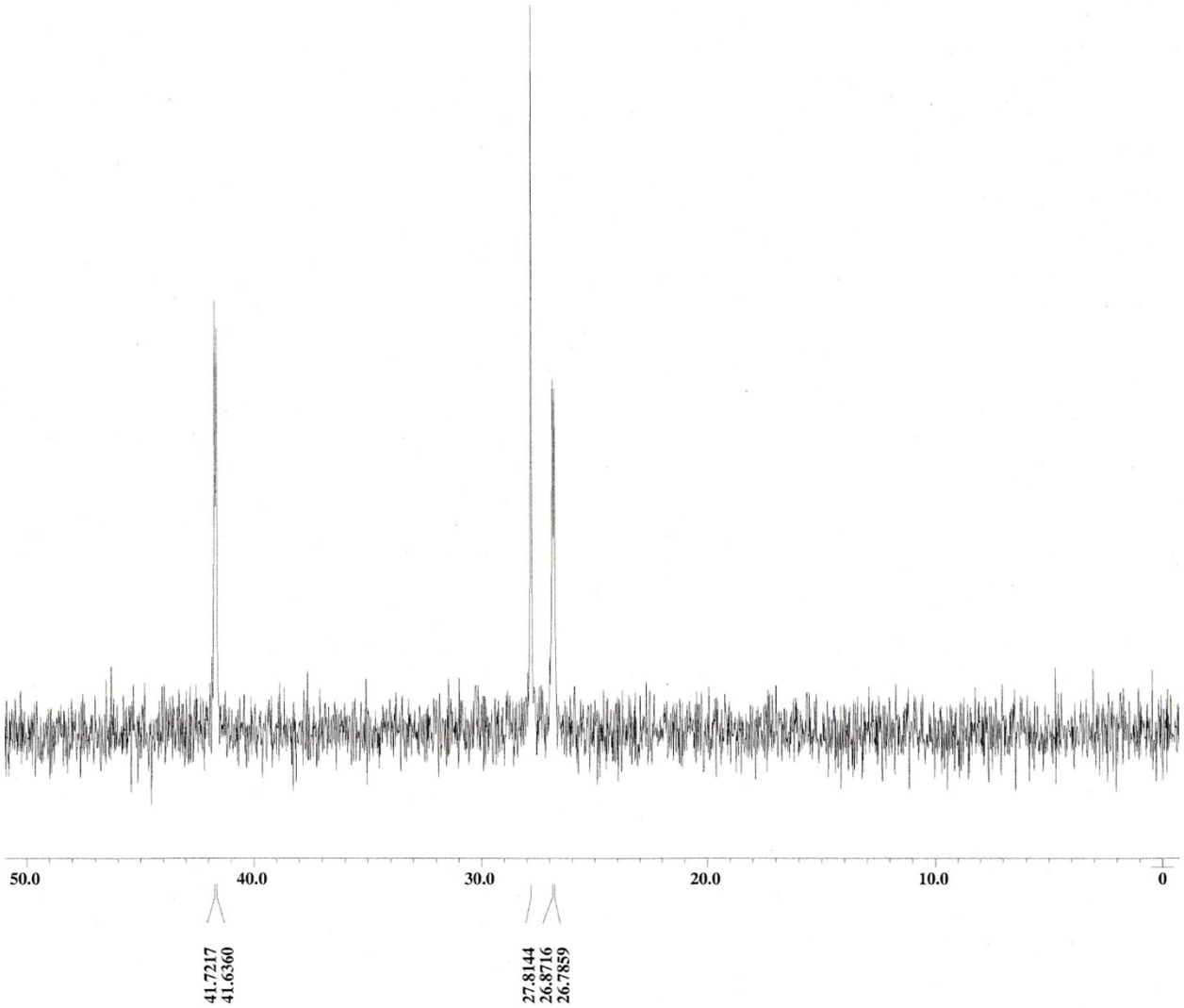


Fig. S30 $^{31}P\{^{1}H\}$ NMR spectrum of $[Pd(dppf)(P(p\text{-}C_6H_4OCH_3)_3)][BF_4]_2$ in CH_3CN.

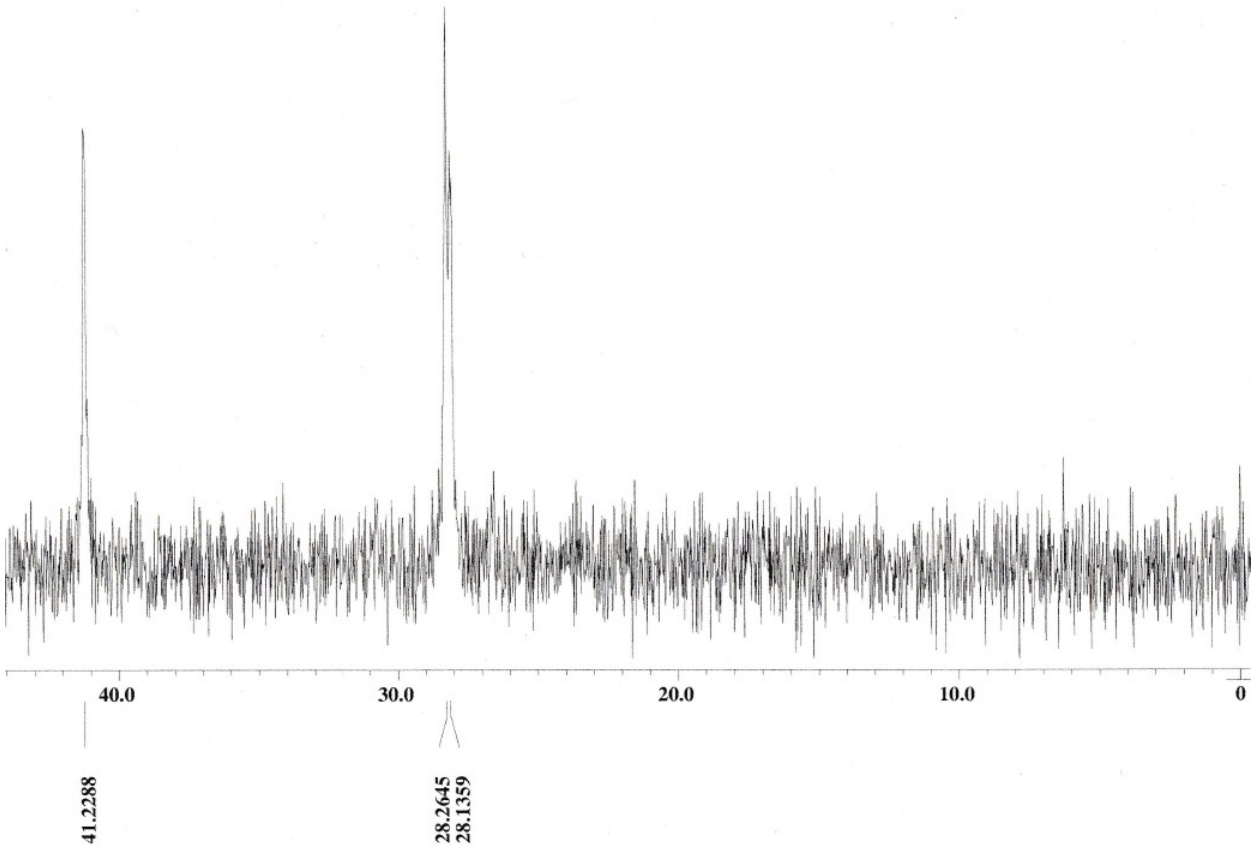


Fig. S31 $^{31}P\{^{1}H\}$ NMR spectrum of $[Pd(dppf)(P(p\text{-}C_6H_4CH_3)_3)][BF_4]_2$ in CH_3CN.

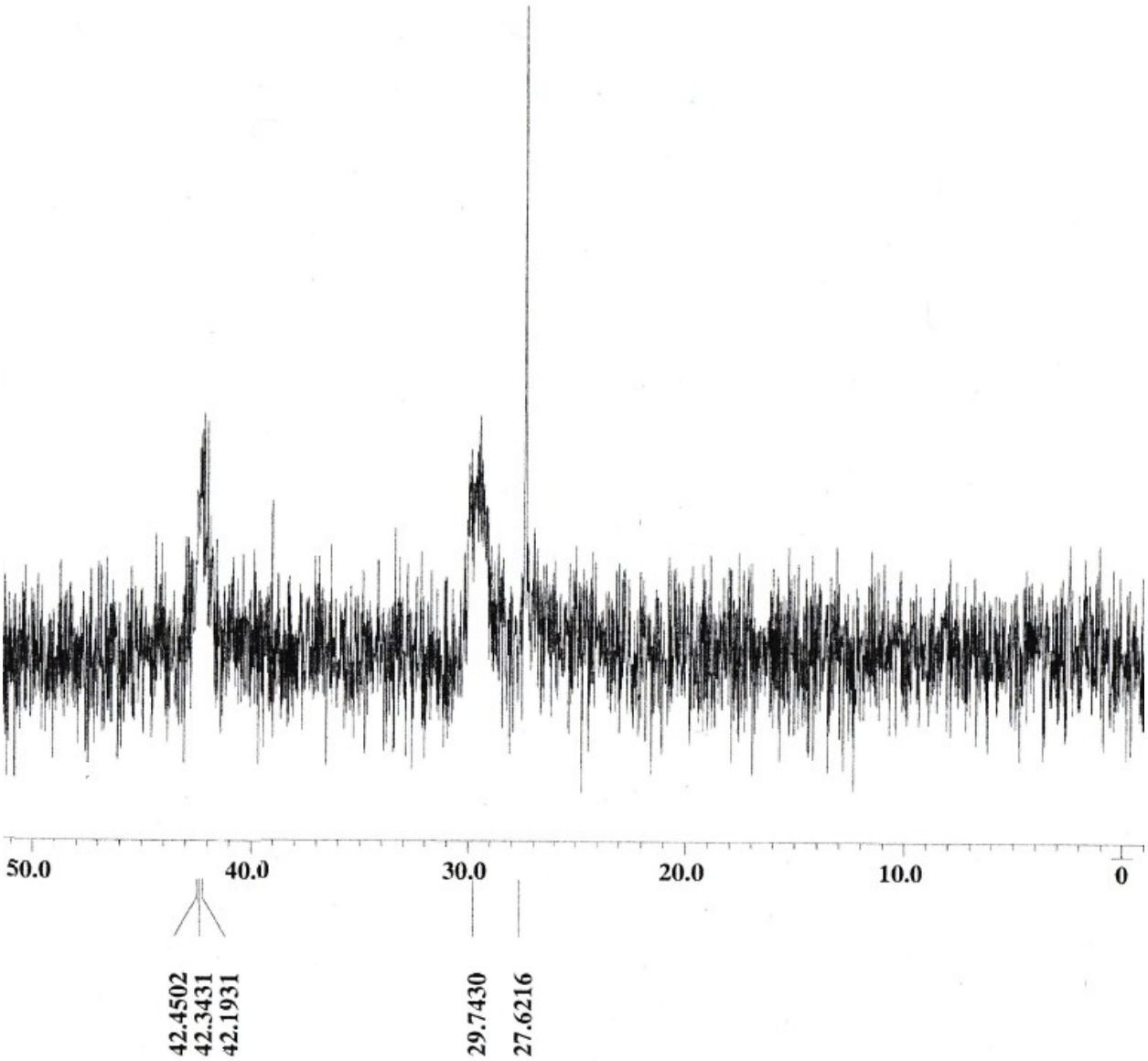


Fig. S32 $^{31}P\{^{1}H\}$ NMR spectrum of $[Pd(dppf)(PPh_3)][BF_4]_2$ in CH_3CN.

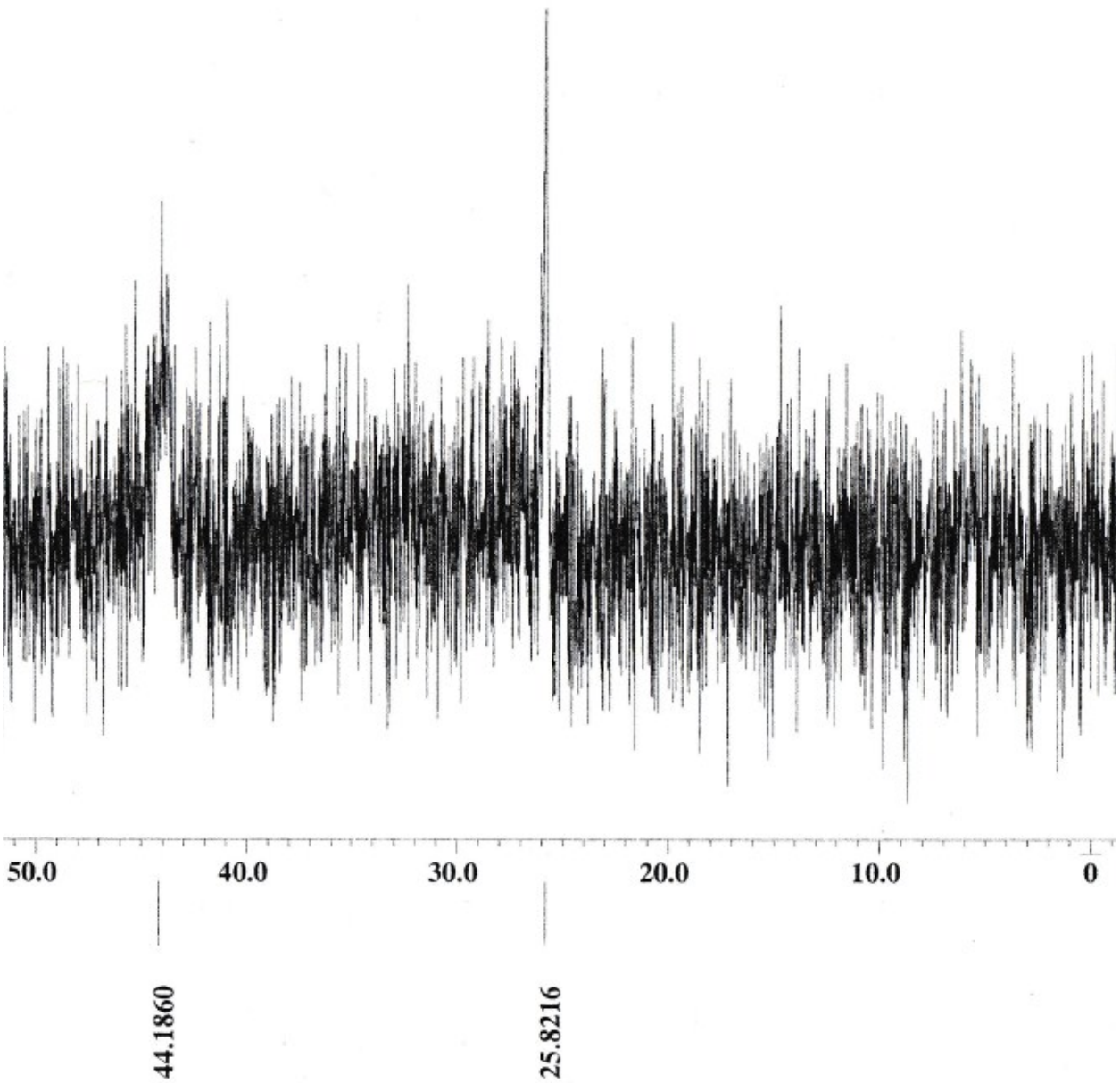


Fig. S33 $^{31}P\{^{1}H\}$ NMR spectrum of $[Pd(dppf)(P(p\text{-}C_6H_4F)_3)][BF_4]_2$ in CH_3CN.

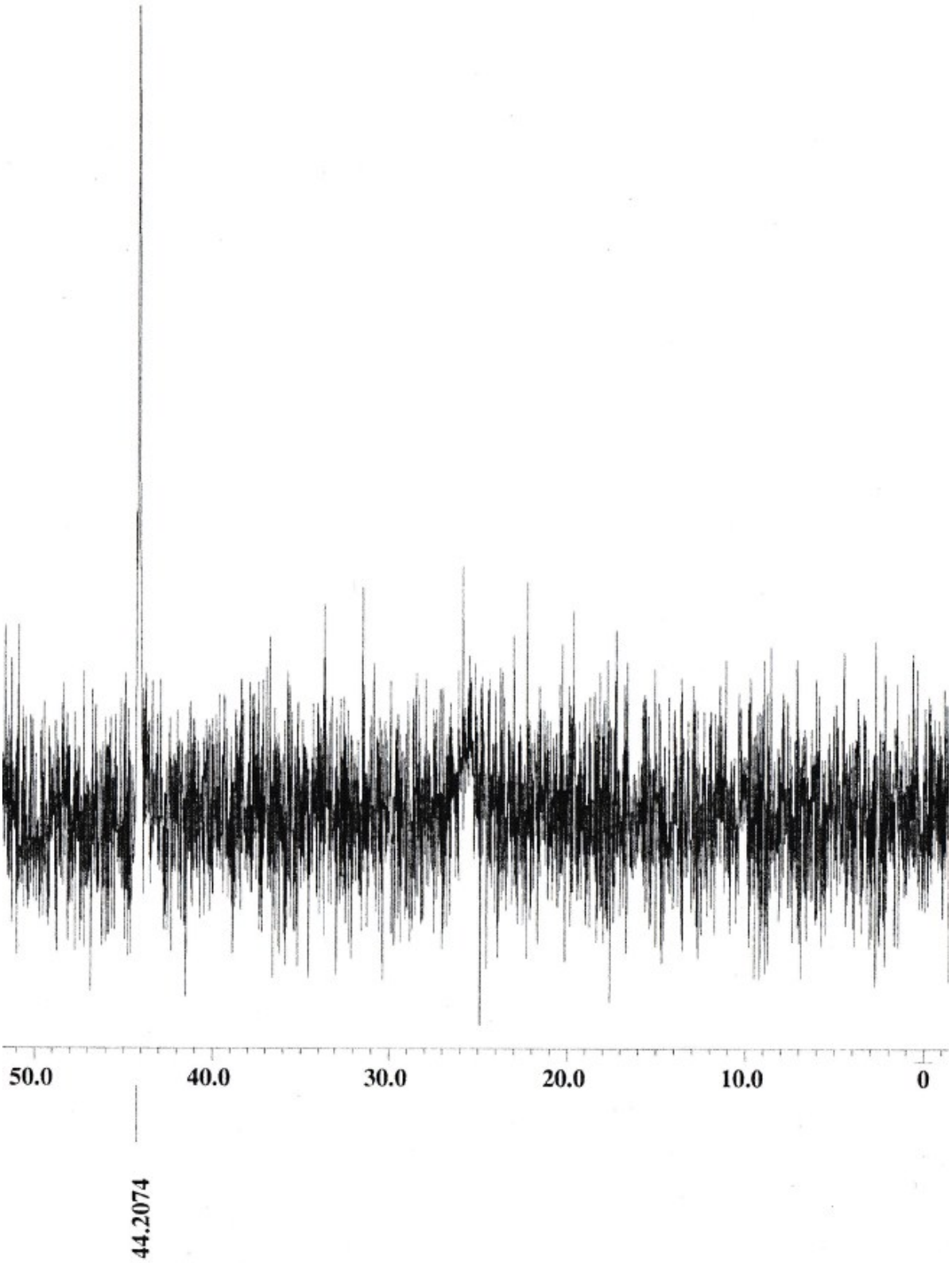


Fig. S34 $^{31}P\{^{1}H\}$ NMR spectrum of $[Pd(dppf)(P(p\text{-}C_6H_4CF_3)_3)][BF_4]_2$ in CH_3CN.

DFT calculations

Table S2 Comparison of geometries from X-ray data and calculations for [Pd(dppf)(P(*p*-$C_6H_4R)_3$)][BF_4]$_2$ (R = CF_3, H, and OCH_3).

	R = CF_3	**R = H**		**R = OCH_3**
Parameter	**Calculated**	**Exp**	**Calculated**	**Calculated**
Fe-Pd (Å)	2.98	2.89	3.00	3.04
Pd-P(1) (Å)	2.40	2.31	2.40	2.39
Pd-P(2) (Å)	2.36	2.28	2.35	2.34
Pd-P(3) (Å)	2.33	2.28	2.33	2.33
P(1)-Pd-Fe (°)	76.0	77.8	75.6	75.6
Fe-Pd-P(2) (°)	77.5	79.1	77.8	77.4
Fe-Pd-P(3) (°)	177.6	178.2	179.3	179.0

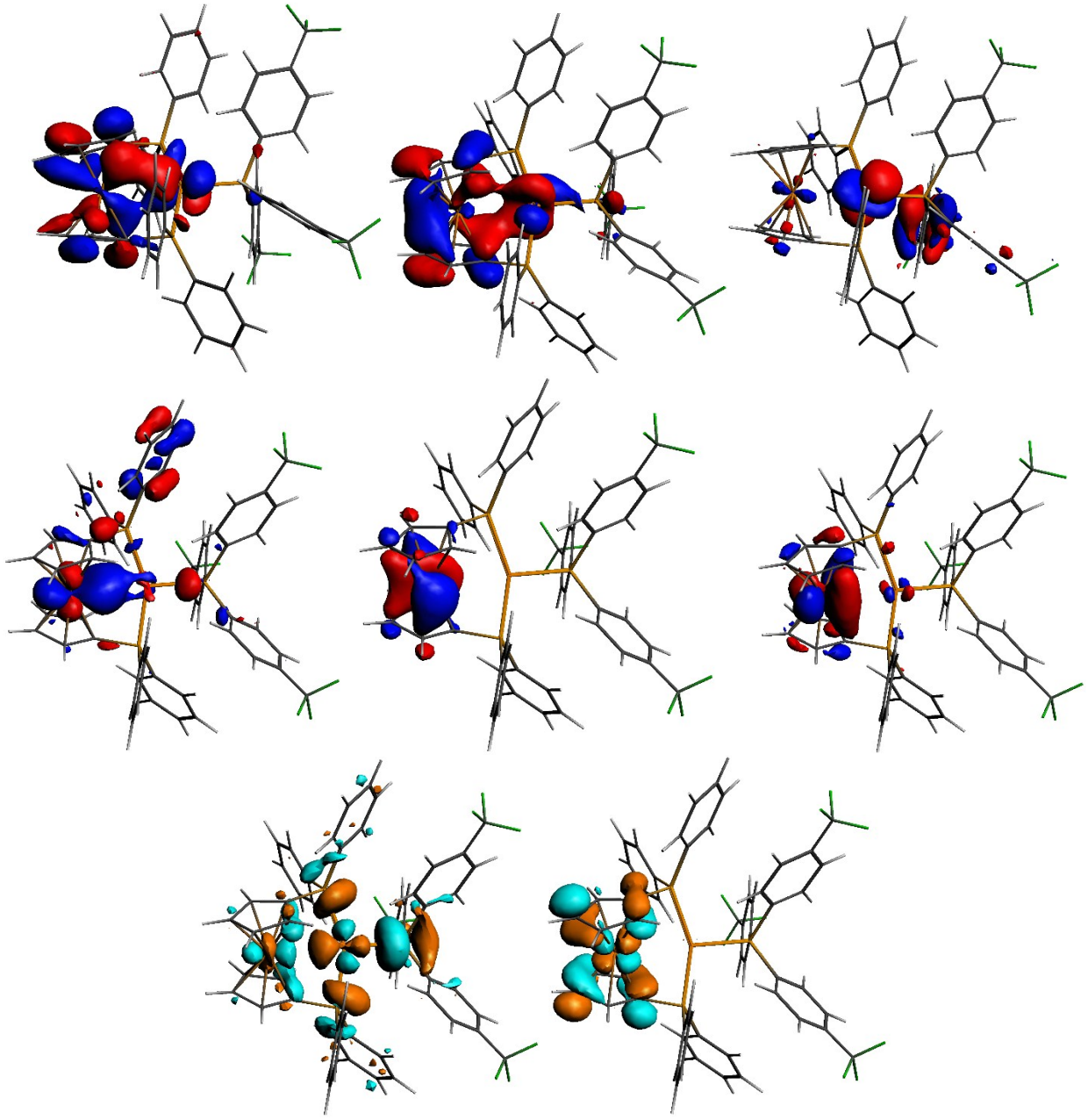


Fig. S35 Frontier molecular orbitals for [Pd(dppf)(P(*p*-$C_6H_4CF_3$)$_3$)][BF_4]$_2$: HOMO-23 (top left), HOMO-22 (top middle), HOMO-17 (top right), HOMO-2 (middle left), HOMO-1 (middle), HOMO (middle right), LUMO (bottom left), LUMO+1 (bottom right); isosurface value = 0.03.

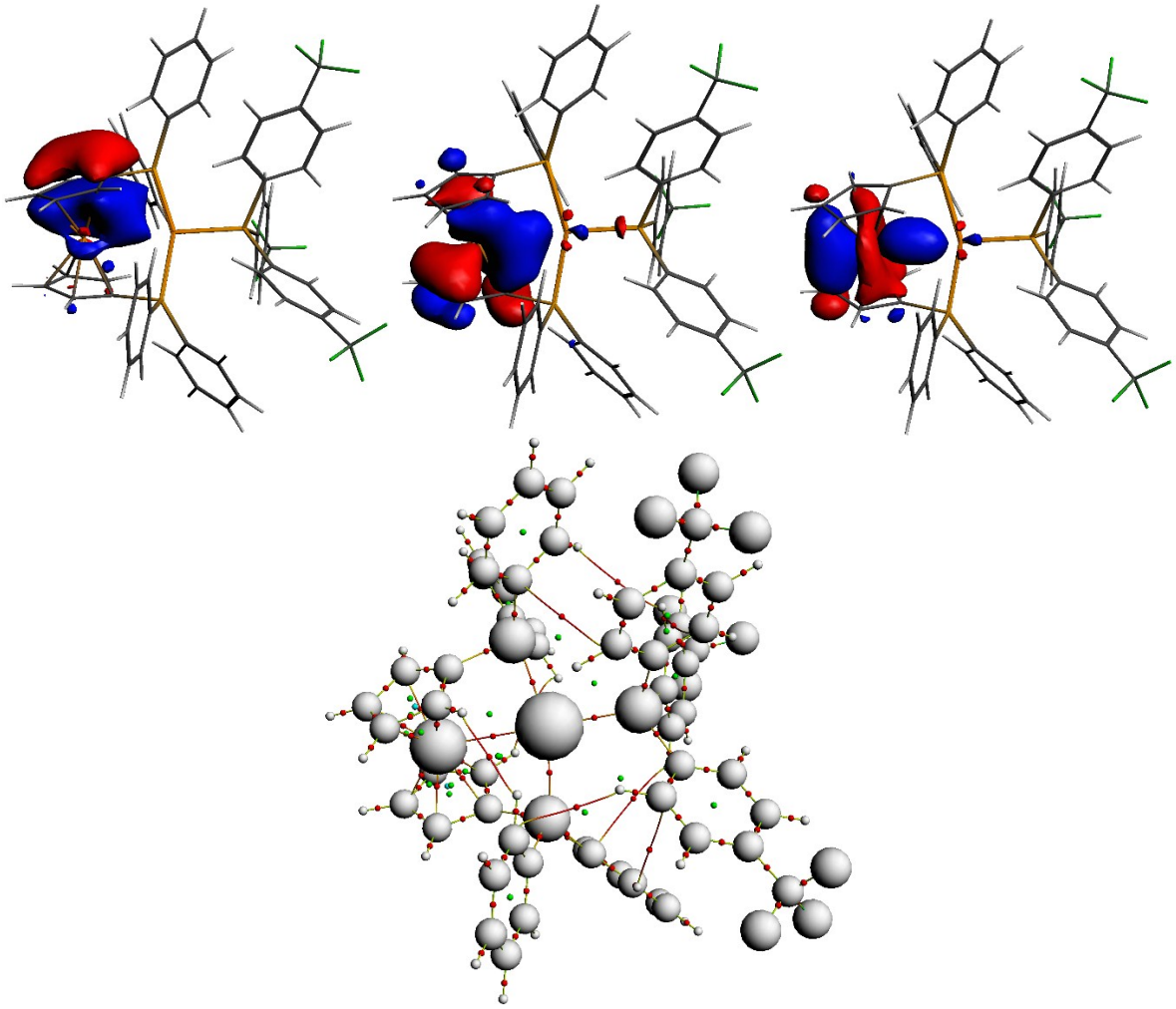


Fig. S36 NLMO 158 (top left), NLMO 111 (top middle), NLMO 109 (top right), and Bader bond critical points (bottom) for [Pd(dppf)(P(*p*-$C_6H_4CF_3$)$_3$)][BF_4]$_2$.

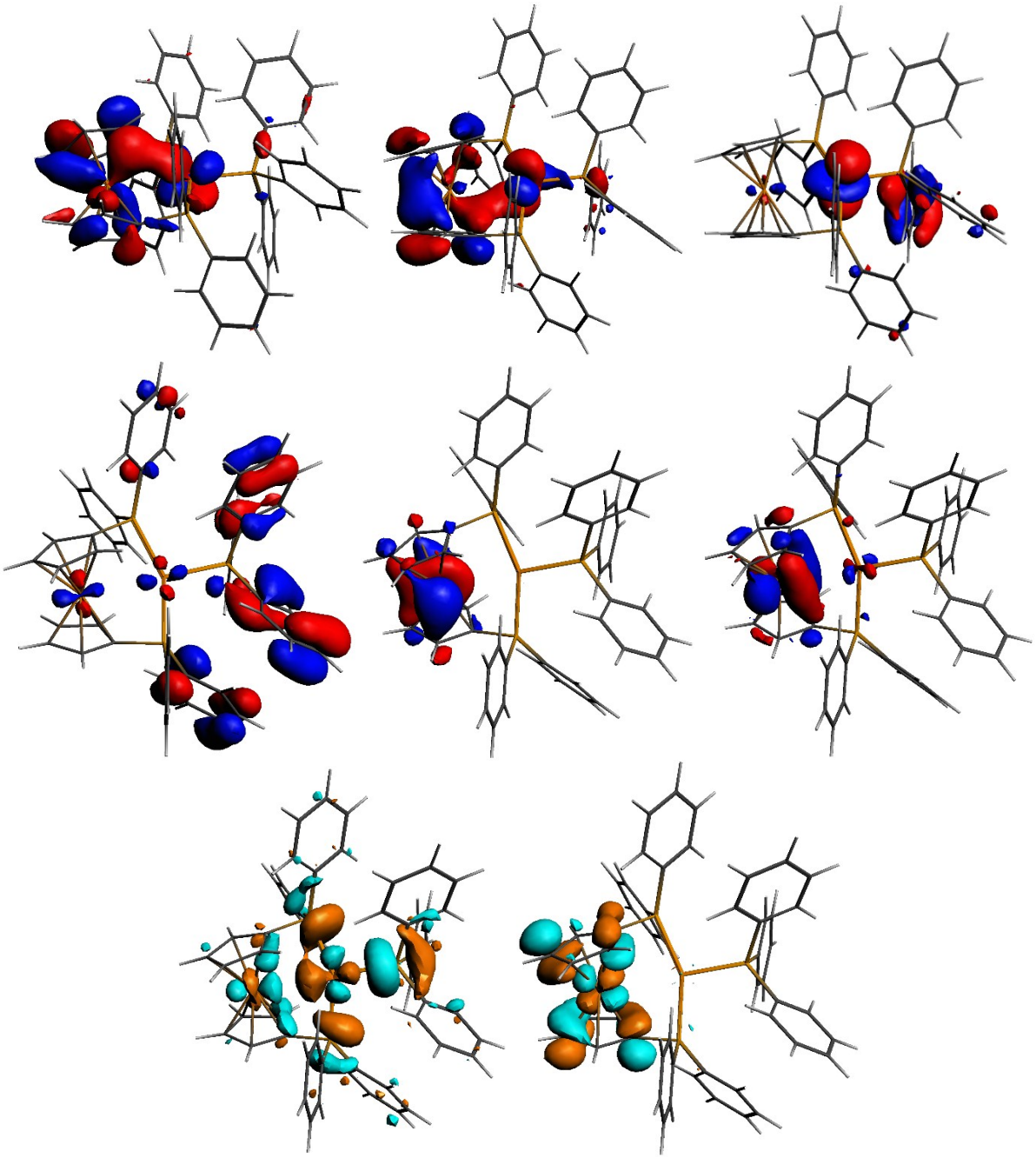


Fig. S37 Frontier molecular orbitals for $[Pd(dppf)(PPh_3)][BF_4]_2$: HOMO-23 (top left), HOMO-22 (top middle), HOMO-17 (top right), HOMO-13 (middle left), HOMO-1 (middle), HOMO (middle right), LUMO (bottom left), LUMO+1 (bottom right); isosurface value = 0.03.

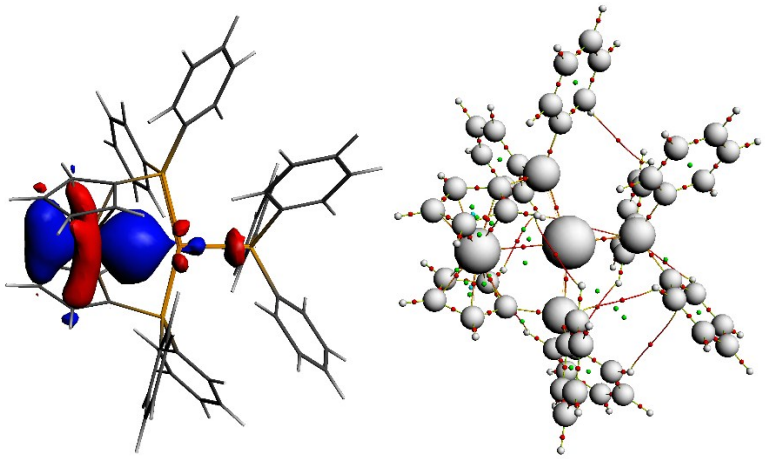


Fig. S38 NLMO 97 (left) and Bader bond critical points (right) for $[Pd(dppf)(PPh_3)][BF_4]_2$.

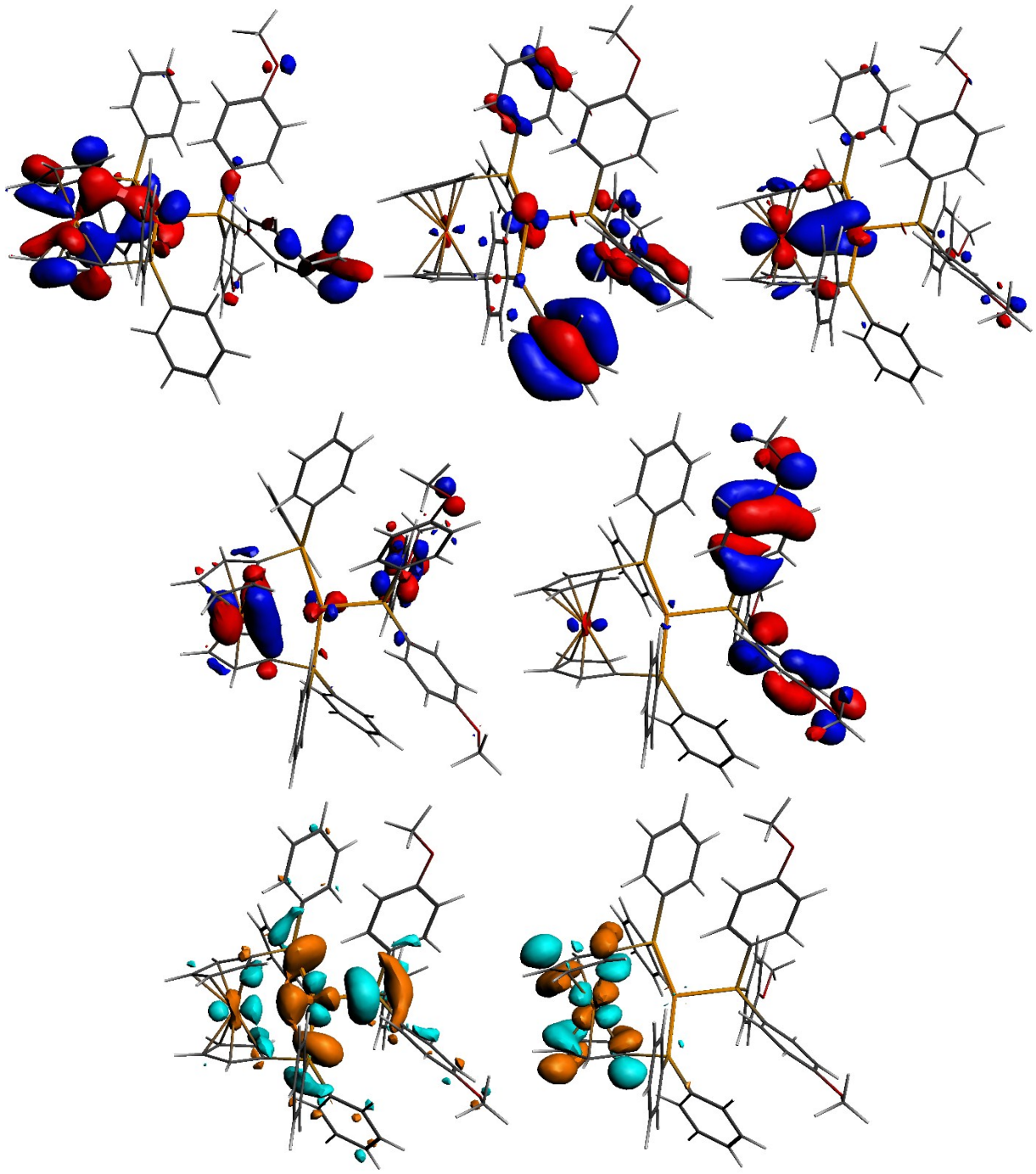


Fig. S39 Frontier molecular orbitals for [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$: HOMO-26 (top left), HOMO-10 (top middle), HOMO-5 (top right), HOMO-1 (middle left), HOMO (middle right), LUMO (bottom left), LUMO+1 (bottom right); isosurface value = 0.03.

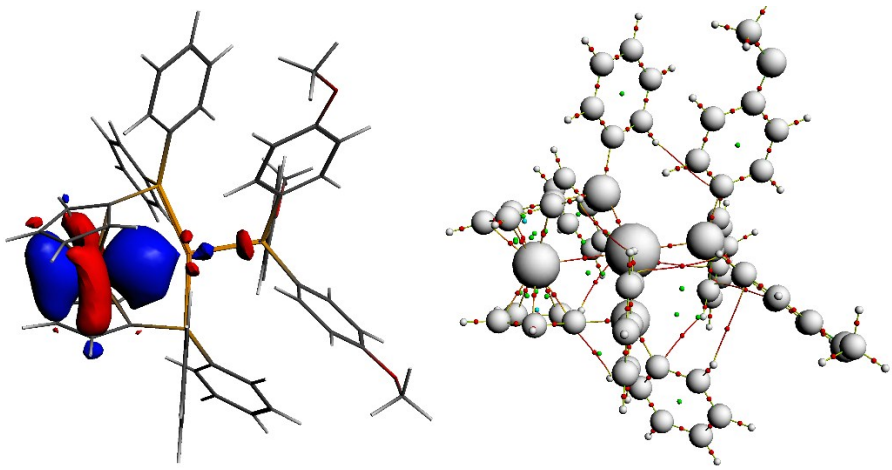


Fig. S40 NLMO 103 (left) and Bader bond critical points (right) for [Pd(dppf)(P(*p*-$C_6H_4OCH_3)_3$)][BF_4]$_2$.

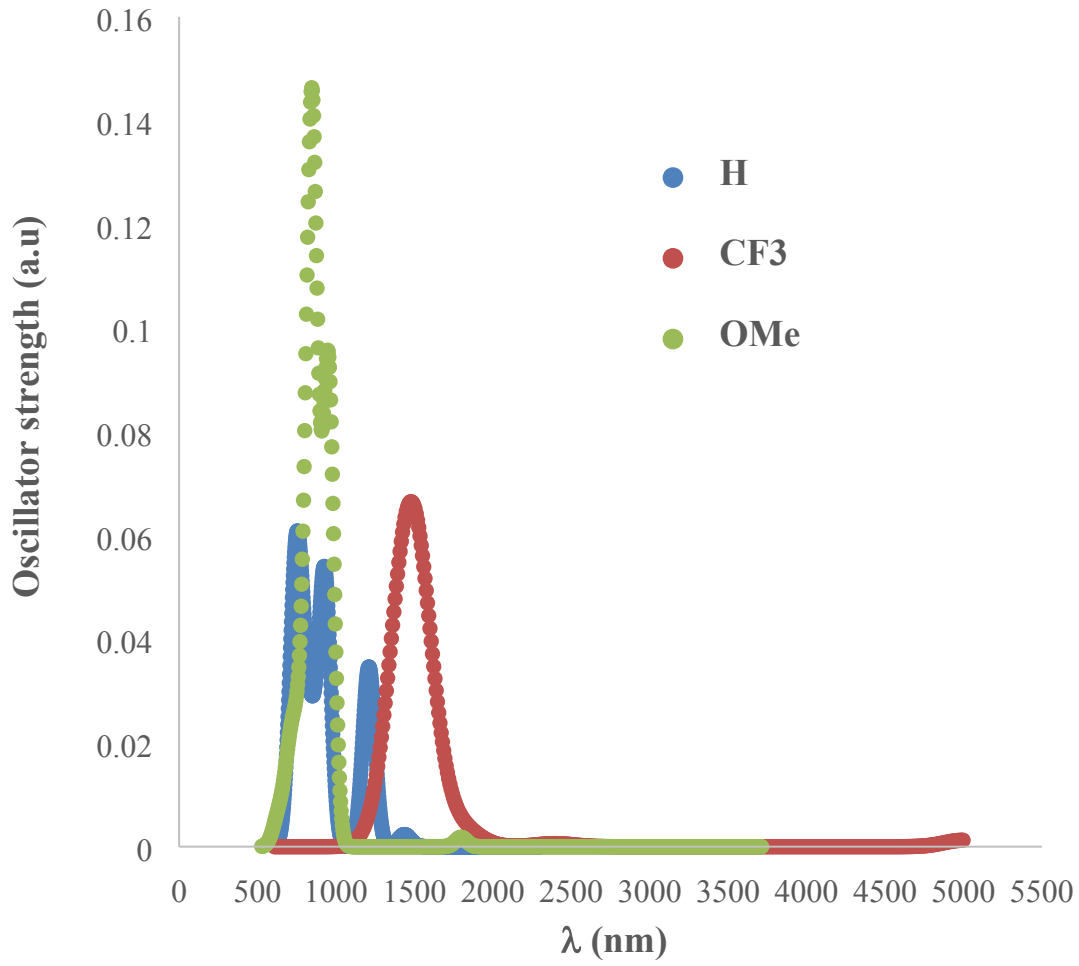


Fig. S41 Calculated spectra for $[Pd(dppf)(P(p\text{-}C_6H_4R)_3)][BF_4]_2$ (R = CF_3, H, or OCH_3).

I. Computational details for [Pd(dppf)(P(*p*-$C_6H_4CF_3)_3$)][BF_4]$_2$

Table S3 Optimized coordinates

1.Fe	2.653335	7.658719	3.424242
2.Pd	3.528821	10.498499	3.576853
3.P	1.346357	10.617866	2.591112
4.P	4.236185	12.714930	3.599535
5.P	5.453653	9.328193	4.297242
6.C	1.025020	9.001983	3.324679
7.C	-0.062285	11.687346	3.020415
8.C	-0.886653	11.402611	4.120455
9.H	-0.740121	10.495367	4.704583
10.C	-1.928533	12.268955	4.449229
11.H	-2.578852	12.033787	5.289814
12.C	-2.149271	13.422533	3.691832
13.H	-2.965602	14.095386	3.949477
14.C	-1.333218	13.704812	2.592373
15.H	-1.515228	14.593897	1.991408
16.C	-0.288361	12.846217	2.257940
17.H	0.330030	13.059247	1.387429
18.C	4.653189	13.125850	1.874182
19.C	3.719198	13.759576	1.039661
20.H	2.783848	14.135422	1.447946
21.C	3.980319	13.904931	-0.319507
22.H	3.252626	14.391300	-0.965890
23.C	5.169854	13.403815	-0.856523
24.F	4.287032	13.320583	-3.056111
25.C	6.112914	12.785385	-0.030593
26.H	7.042480	12.407348	-0.451656
27.C	5.854926	12.639766	1.329878
28.H	6.587486	12.141079	1.962135
29.C	5.690610	13.114236	4.638747
30.C	5.699847	12.629074	5.954794
31.H	4.927482	11.941402	6.293526
32.C	6.687628	13.033422	6.848055
33.H	6.690922	12.659612	7.869739
34.C	7.676855	13.925155	6.423484
35.F	9.970149	14.417406	6.804499
36.C	7.672893	14.416763	5.113777
37.H	8.443149	15.115417	4.790760
38.C	6.679708	14.017207	4.221397
39.H	6.677800	14.418805	3.210862
40.C	2.022673	13.480001	5.117367
41.H	1.966894	12.430058	5.401217

42.C	1.131493	14.393715	5.675533
43.H	0.383202	14.065713	6.393707
44.C	1.196224	15.735439	5.300331
45.F	0.822232	17.796026	6.420597
46.C	2.170926	16.175441	4.394884
47.H	2.230104	17.228032	4.123627
48.C	3.072751	15.266298	3.852843
49.H	3.840441	15.619697	3.168851
50.C	7.128446	9.590908	3.627585
51.C	8.056287	10.329167	4.382206
52.H	7.796293	10.689825	5.375406
53.C	9.328873	10.577226	3.871460
54.H	10.047198	11.134381	4.470414
55.C	9.682044	10.107450	2.604081
56.H	10.679117	10.298011	2.210690
57.C	8.761219	9.375404	1.849918
58.H	9.041178	8.986133	0.872714
59.C	7.487803	9.116848	2.353792
60.H	6.795266	8.519948	1.764478
61.C	4.767745	7.867312	3.493366
62.C	4.294272	7.835423	2.115194
63.H	4.436735	8.607753	1.369491
64.C	3.654335	6.588177	1.903146
65.H	3.202276	6.256140	0.974501
66.C	3.693800	5.857617	3.133866
67.H	3.281858	4.867205	3.295494
68.C	4.368025	6.641636	4.115662
69.H	4.554844	6.362033	5.147341
70.C	5.614800	8.880989	6.052914
71.C	4.588517	9.222160	6.948700
72.H	3.734128	9.798876	6.596197
73.C	4.662713	8.825632	8.282490
74.H	3.868716	9.095392	8.977144
75.C	5.764862	8.091639	8.729230
76.H	5.827444	7.786913	9.772677
77.C	6.788899	7.751143	7.841148
78.H	7.647040	7.179586	8.189208
79.C	6.720951	8.145491	6.504810
80.H	7.522074	7.880065	5.817897
81.C	1.277399	10.371393	0.790678
82.C	2.462710	10.326541	0.041209
83.H	3.419483	10.509533	0.529874
84.C	2.412784	10.079486	-1.329950
85.H	3.332542	10.057715	-1.912430

86.C	1.181288	9.878606	-1.957858
87.H	1.142096	9.691126	-3.029717
88.C	-0.003188	9.935684	-1.216719
89.H	-0.963489	9.790426	-1.708235
90.C	0.038423	10.185580	0.153715
91.H	-0.886938	10.241266	0.724707
92.C	1.335186	8.687858	4.714443
93.H	1.592658	9.405020	5.485650
94.C	1.170845	7.291595	4.896821
95.H	1.323968	6.745989	5.822078
96.C	0.781010	6.729092	3.639643
97.H	0.582799	5.678559	3.452273
98.C	0.693964	7.773858	2.670672
99.H	0.433691	7.660953	1.623514
100.C	2.985177	13.906027	4.194186
101.C	0.200737	16.737461	5.842878
102.F	-0.582277	17.230110	4.838766
103.F	-0.628980	16.188412	6.769016
104.C	8.739357	14.405158	7.389324
105.F	8.480359	15.669127	7.809967
106.F	8.818314	13.612409	8.490874
107.C	5.425548	13.543506	-2.341437
108.F	5.863964	14.785779	-2.661410
109.F	6.358873	12.652123	-2.774704

Table S4 Selected individual LMO bond orders greater than 0.002 in magnitude, with the overlap between the hybrids in the NLMO given:

Atom I	Atom J	NLMO	Bond Order	Hybrid Overlap
1	2	107	0.0041630	0.0250830
1	2	109	0.0358336	0.1298277
1	2	110	0.0163781	0.0068655
1	2	111	0.0634562	0.1012067
1	2	117	0.0038764	0.0092515
1	2	146	0.0022793	0.1293446
1	2	158	0.0222342	0.2376691
1	2	230	0.0124288	0.1959526
1	2	232	-0.0105496	-0.0098055
1	2	268	-0.0031340	-0.0066099

Table S5 Natural localized molecular orbital (NLMO) analysis for NLMOs with a bond order greater than 0.02:

Hybridization/Polarization Analysis of NLMOs in NAO Basis:

NLMO/Occupancy/Percent from Parent NBO/ Atomic Hybrid Contributions

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109. (2.00000) 76.4953% LP (3)Fe 1
78.358% Fe 1 s(0.35%)p 0.05(0.02%)d99.99(99.64%)
1.792% Pd 2 s(21.89%)p 0.04(0.79%)d 3.53(77.32%)
0.398% P 3 s(21.96%)p 3.46(75.95%)d 0.10(2.09%)
0.994% P 4 s(41.27%)p 1.42(58.66%)d 0.00(0.06%)
0.734% P 5 s(23.57%)p 3.21(75.73%)d 0.03(0.71%)
0.051% C 6 s(0.60%)p99.99(79.19%)d33.70(20.21%)
0.036% C 7 s(30.05%)p 2.31(69.39%)d 0.02(0.56%)
0.032% C 13 s(6.88%)p13.48(92.68%)d 0.06(0.44%)
0.013% C 14 s(1.70%)p57.62(98.06%)d 0.14(0.24%)
0.013% C 18 s(1.44%)p68.16(98.27%)d 0.20(0.29%)
0.019% C 19 s(15.83%)p 5.26(83.23%)d 0.06(0.94%)
0.095% C 30 s(1.59%)p61.76(98.32%)d 0.06(0.09%)
0.073% C 31 s(0.13%)p99.99(99.83%)d 0.28(0.04%)
0.031% C 33 s(0.03%)p99.99(99.97%)d 0.25(0.01%)
0.077% C 35 s(0.26%)p99.99(99.71%)d 0.11(0.03%)
1.131% C 36 s(0.44%)p99.99(98.85%)d 1.59(0.70%)
1.262% C 37 s(1.23%)p79.85(98.45%)d 0.26(0.32%)
0.524% C 38 s(0.62%)p99.99(96.67%)d 4.37(2.71%)
8.963% C 39 s(1.46%)p67.24(98.45%)d 0.06(0.09%)
0.600% C 40 s(2.09%)p46.33(96.69%)d 0.58(1.22%)
0.012% C 41 s(28.70%)p 2.37(67.93%)d 0.12(3.37%)
0.089% C 53 s(1.40%)p65.28(91.14%)d 5.35(7.47%)
0.039% C 54 s(17.70%)p 3.69(65.33%)d 0.96(16.97%)
3.763% C 55 s(3.40%)p28.35(96.49%)d 0.03(0.10%)
0.744% C 56 s(1.45%)p67.73(97.91%)d 0.44(0.64%)
0.015% C 57 s(24.25%)p 3.06(74.24%)d 0.06(1.51%)
0.017% H 99 s(81.20%)p 0.23(18.80%)

110. (2.00000) 36.5453% LP (4)Fe 1
36.829% Fe 1 s(0.13%)p 1.51(0.20%)d99.99(99.67%)
0.819% Pd 2 s(32.71%)p 0.05(1.63%)d 2.01(65.67%)
0.358% P 3 s(1.17%)p71.26(83.27%)d13.31(15.56%)
0.662% P 4 s(34.66%)p 1.88(65.28%)d 0.00(0.06%)
0.246% P 5 s(14.92%)p 5.63(84.02%)d 0.07(1.06%)
7.442% C 6 s(0.01%)p 1.00(99.84%)d 0.00(0.15%)
0.159% C 7 s(43.63%)p 1.28(55.81%)d 0.01(0.55%)
0.023% C 8 s(60.90%)p 0.63(38.55%)d 0.01(0.55%)

0.012% C 13 s(15.30%)p 5.51(84.32%)d 0.02(0.38%)
0.036% C 30 s(7.81%)p11.78(91.99%)d 0.03(0.20%)
0.021% C 31 s(0.76%)p99.99(99.20%)d 0.06(0.04%)
0.019% C 35 s(0.65%)p99.99(99.30%)d 0.08(0.05%)
0.062% C 36 s(43.23%)p 1.30(56.04%)d 0.02(0.74%)
0.083% C 37 s(8.38%)p10.86(90.97%)d 0.08(0.65%)
0.044% C 38 s(40.90%)p 1.35(55.12%)d 0.10(3.97%)
0.105% C 39 s(35.50%)p 1.72(61.07%)d 0.10(3.43%)
0.070% C 40 s(7.92%)p11.42(90.49%)d 0.20(1.59%)
0.011% C 47 s(30.83%)p 2.20(67.76%)d 0.05(1.41%)
5.827% C 53 s(0.79%)p99.99(99.06%)d 0.20(0.15%)
7.524% C 54 s(1.47%)p66.86(98.15%)d 0.26(0.38%)
32.372% C 55 s(1.84%)p53.27(98.04%)d 0.07(0.12%)
7.106% C 56 s(1.45%)p67.75(98.15%)d 0.28(0.40%)
0.014% H 61 s(91.88%)p 0.09(8.12%)
0.025% H 85 s(98.04%)p 0.02(1.96%)
111. (2.00000) 15.3780% LP (5)Fe 1
31.278% Fe 1 s(0.92%)p 0.36(0.33%)d99.99(98.76%)
3.173% Pd 2 s(25.86%)p 0.04(1.11%)d 2.82(73.03%)
0.555% P 3 s(5.07%)p18.24(92.52%)d 0.47(2.41%)
2.427% P 4 s(30.35%)p 2.29(69.58%)d 0.00(0.07%)
0.592% P 5 s(0.97%)p87.89(85.57%)d13.82(13.46%)
0.230% C 6 s(19.20%)p 3.99(76.53%)d 0.22(4.27%)
0.077% C 7 s(28.61%)p 2.48(71.03%)d 0.01(0.35%)
0.023% C 8 s(18.36%)p 4.44(81.53%)d 0.01(0.11%)
0.025% C 10 s(0.85%)p99.99(99.14%)d 0.01(0.01%)
0.013% C 12 s(3.35%)p28.81(96.56%)d 0.03(0.09%)
0.014% C 13 s(40.76%)p 1.44(58.50%)d 0.02(0.74%)
0.065% C 14 s(0.81%)p99.99(99.15%)d 0.05(0.04%)
0.044% C 16 s(0.07%)p99.99(99.91%)d 0.36(0.02%)
0.040% C 18 s(1.00%)p98.87(98.89%)d 0.11(0.11%)
0.035% C 19 s(26.50%)p 2.75(72.85%)d 0.02(0.66%)
0.031% C 20 s(10.69%)p 8.35(89.21%)d 0.01(0.10%)
0.022% C 22 s(0.59%)p99.99(99.38%)d 0.05(0.03%)
0.037% C 24 s(18.69%)p 4.33(80.97%)d 0.02(0.34%)
0.011% C 25 s(36.71%)p 1.72(63.16%)d 0.00(0.13%)
0.043% C 29 s(30.11%)p 2.31(69.50%)d 0.01(0.39%)
0.667% C 30 s(19.70%)p 4.06(80.08%)d 0.01(0.22%)
0.137% C 31 s(1.82%)p53.87(98.05%)d 0.07(0.13%)
0.018% C 32 s(20.08%)p 3.94(79.17%)d 0.04(0.75%)
0.093% C 33 s(1.74%)p56.46(98.24%)d 0.01(0.02%)
0.135% C 35 s(14.19%)p 6.03(85.62%)d 0.01(0.19%)
10.527% C 36 s(0.49%)p99.99(99.28%)d 0.48(0.23%)
17.618% C 37 s(1.21%)p81.49(98.72%)d 0.06(0.07%)

0.305% C 38 s(37.33%)p 1.57(58.55%)d 0.11(4.13%)
14.683% C 39 s(1.35%)p72.89(98.55%)d 0.07(0.10%)
6.758% C 40 s(3.49%)p27.56(96.28%)d 0.07(0.23%)
0.039% C 41 s(23.46%)p 3.23(75.72%)d 0.04(0.82%)
0.011% C 46 s(15.86%)p 5.28(83.78%)d 0.02(0.36%)
0.024% C 47 s(29.59%)p 2.34(69.27%)d 0.04(1.14%)
0.012% C 48 s(13.22%)p 6.52(86.15%)d 0.05(0.62%)
0.014% C 52 s(29.15%)p 2.42(70.56%)d 0.01(0.29%)
3.597% C 53 s(2.78%)p35.00(97.19%)d 0.01(0.03%)
0.397% C 54 s(4.69%)p20.24(94.83%)d 0.10(0.49%)
1.921% C 55 s(6.65%)p14.02(93.20%)d 0.02(0.16%)
4.114% C 56 s(1.38%)p71.13(98.50%)d 0.09(0.12%)
0.038% C 57 s(16.15%)p 5.14(82.97%)d 0.05(0.88%)
0.027% H 82 s(94.61%)p 0.06(5.39%)
0.014% H 86 s(98.90%)p 0.01(1.10%)
0.017% H 97 s(95.42%)p 0.05(4.58%)
158. (2.00000) 74.1673% BD (2) C 6- C 56
8.411% Fe 1 s(26.67%)p 0.04(1.17%)d 2.71(72.16%)
1.112% Pd 2 s(29.58%)p 0.05(1.56%)d 2.33(68.85%)
1.095% P 3 s(0.42%)p99.99(88.85%)d25.66(10.74%)
0.830% P 4 s(32.89%)p 2.04(66.97%)d 0.00(0.14%)
0.224% P 5 s(23.24%)p 3.23(75.05%)d 0.07(1.71%)
42.553% C 6 s(1.01%)p97.52(98.89%)d 0.10(0.10%)
0.328% C 7 s(41.16%)p 1.41(58.12%)d 0.02(0.72%)
0.037% C 8 s(27.74%)p 2.56(70.89%)d 0.05(1.37%)
0.012% C 10 s(16.24%)p 5.15(83.63%)d 0.01(0.12%)
0.028% C 12 s(24.55%)p 3.06(75.20%)d 0.01(0.25%)
0.019% C 14 s(0.46%)p99.99(99.50%)d 0.09(0.04%)
0.011% C 18 s(1.19%)p82.71(98.72%)d 0.07(0.08%)
0.057% C 30 s(4.15%)p23.10(95.77%)d 0.02(0.09%)
0.029% C 31 s(0.08%)p99.99(99.86%)d 0.90(0.07%)
0.017% C 33 s(0.19%)p99.99(99.80%)d 0.03(0.01%)
0.029% C 35 s(3.34%)p28.93(96.60%)d 0.02(0.06%)
0.274% C 36 s(1.69%)p57.50(97.45%)d 0.50(0.86%)
2.139% C 37 s(2.56%)p37.99(97.37%)d 0.03(0.07%)
0.425% C 38 s(11.97%)p 7.32(87.60%)d 0.04(0.43%)
0.666% C 39 s(1.31%)p75.48(98.50%)d 0.15(0.19%)
1.197% C 40 s(1.40%)p70.47(98.52%)d 0.06(0.08%)
0.050% C 47 s(33.37%)p 1.95(65.08%)d 0.05(1.55%)
0.027% C 52 s(3.36%)p28.65(96.26%)d 0.11(0.38%)
4.080% C 53 s(2.82%)p34.27(96.60%)d 0.21(0.58%)
0.124% C 54 s(18.22%)p 4.20(76.59%)d 0.29(5.20%)
4.312% C 55 s(2.41%)p40.31(96.97%)d 0.26(0.62%)
31.694% C 56 s(2.41%)p40.37(97.41%)d 0.07(0.17%)

0.010% C 57 s(30.58%)p 2.24(68.38%)d 0.03(1.03%)
0.044% H 61 s(99.17%)p 0.01(0.83%)
0.010% H 83 s(98.91%)p 0.01(1.09%)
0.010% H 84 s(98.90%)p 0.01(1.10%)

Table S6 List of selected MOs, ordered by energy, with the most significant SFO gross populations

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-12.592	2.00	260 A	22.55%	2 D:yz	-4.129	2.00	2 Pd
			7.98%	1 D:xy	-7.605	1.20	1 Fe
			7.66%	2 D:xz	-4.129	2.00	2 Pd
			7.55%	1 P:x	-5.339	0.67	53 C
			5.22%	1 P:x	-5.339	0.67	55 C
			4.21%	1 P:x	-5.339	0.67	37 C
			3.89%	1 P:x	-5.339	0.67	56 C
			2.33%	1 P:x	-5.339	0.67	39 C
			2.17%	1 D:x2-y2	-7.605	1.20	1 Fe
			1.61%	1 D:yz	-7.605	1.20	1 Fe
			1.57%	1 P:x	-5.339	0.67	40 C
			1.48%	2 P:x	-5.563	1.00	3 P
			1.46%	3 P:z	-0.725	0.00	1 Fe
			1.28%	1 P:y	-5.339	0.67	40 C
			1.23%	2 P:y	-5.563	1.00	5 P
			1.19%	2 D:z2	-4.129	2.00	2 Pd
-12.497	2.00	261 A	12.44%	2 D:xz	-4.129	2.00	2 Pd
			11.65%	2 D:yz	-4.129	2.00	2 Pd
			8.25%	1 P:x	-5.339	0.67	39 C
			7.90%	1 P:x	-5.339	0.67	55 C
			4.66%	1 P:x	-5.339	0.67	37 C
			4.40%	1 P:x	-5.339	0.67	36 C
			4.31%	1 P:x	-5.339	0.67	6 C
			3.56%	1 P:x	-5.339	0.67	53 C
			3.37%	3 P:y	-0.725	0.00	1 Fe
			2.96%	2 D:z2	-4.129	2.00	2 Pd
			1.95%	1 P:y	-5.339	0.67	39 C
			1.89%	1 D:x2-y2	-7.605	1.20	1 Fe
			1.70%	1 D:xz	-7.605	1.20	1 Fe
			1.66%	2 P:y	-5.563	1.00	4 P
			1.22%	1 P:x	-5.339	0.67	40 C
			1.14%	2 D:x2-y2	-4.129	2.00	2 Pd
			1.07%	1 P:z	-5.339	0.67	13 C
-12.366	2.00	262 A	19.45%	2 D:x2-y2	-4.129	2.00	2 Pd
			9.44%	2 D:xy	-4.129	2.00	2 Pd
			6.79%	2 D:yz	-4.129	2.00	2 Pd
			4.33%	2 D:z2	-4.129	2.00	2 Pd
			3.82%	1 P:x	-5.339	0.67	6 C
			3.41%	1 P:x	-5.339	0.67	55 C

			1.90%	2 P:x	-5.563	1.00	3 P		
			1.86%	2 P:x	-5.563	1.00	5 P		
			1.77%	1 P:x	-5.339	0.67	54 C		
			1.55%	1 P:x	-5.339	0.67	19 C		
			1.39%	1 P:x	-5.339	0.67	30 C		
			1.37%	2 D:xz	-4.129	2.00	2 Pd		
			1.17%	2 P:z	-5.563	1.00	3 P		
			1.17%	1 P:z	-5.339	0.67	47 C		
			1.15%	3 P:y	-0.725	0.00	1 Fe		
-12.284	2.00	263 A	20.81%	2 D:xy	-4.129	2.00	2 Pd		
			17.86%	2 D:z2	-4.129	2.00	2 Pd		
			17.39%	2 D:xz	-4.129	2.00	2 Pd		
			3.11%	1 P:x	-5.339	0.67	38 C		
			2.95%	1 P:x	-5.339	0.67	36 C		
			1.54%	1 P:y	-5.339	0.67	36 C		
			1.53%	1 P:x	-5.339	0.67	56 C		
			1.53%	1 P:z	-5.339	0.67	41 C		
			1.47%	1 P:x	-5.339	0.67	39 C		
			1.28%	1 P:x	-5.339	0.67	40 C		
			1.24%	1 P:x	-5.339	0.67	53 C		
-12.135	2.00	264 A	17.29%	2 D:yz	-4.129	2.00	2 Pd		
			8.40%	2 D:xz	-4.129	2.00	2 Pd		
			6.63%	2 D:x2-y2	-4.129	2.00	2 Pd		
			5.30%	2 D:xy	-4.129	2.00	2 Pd		
			5.03%	1 D:x2-y2	-7.605	1.20	1 Fe		
			4.18%	1 D:xy	-7.605	1.20	1 Fe		
			3.37%	1 P:y	-5.339	0.67	16 C		
			2.60%	2 P:y	-5.563	1.00	5 P		
			2.34%	1 P:x	-5.339	0.67	39 C		
			2.26%	1 P:y	-5.339	0.67	13 C		
			2.22%	2 P:x	-5.563	1.00	3 P		
			1.87%	1 P:z	-5.339	0.67	13 C		
			1.70%	1 P:x	-5.339	0.67	36 C		
			1.52%	1 P:x	-5.339	0.67	37 C		
			1.30%	1 P:y	-5.339	0.67	17 C		
			1.23%	1 P:y	-5.339	0.67	15 C		
			1.15%	1 P:x	-5.339	0.67	53 C		
-12.017	2.00	265 A	9.21%	1 P:x	-5.339	0.67	54 C		
			9.17%	1 P:x	-5.339	0.67	56 C		
			7.08%	1 P:x	-5.339	0.67	40 C		
			5.76%	1 P:x	-5.339	0.67	38 C		
			4.35%	2 D:yz	-4.129	2.00	2 Pd		
			4.20%	2 D:z2	-4.129	2.00	2 Pd		
			3.97%	3 P:z	-0.725	0.00	1 Fe		

				3.52%	1 P:x	-5.339	0.67	6 C	
				2.60%	1 P:x	-5.339	0.67	37 C	
				2.17%	1 D:yz	-7.605	1.20	1 Fe	
				2.14%	2 P:x	-5.563	1.00	3 P	
				2.12%	1 P:x	-5.339	0.67	53 C	
				1.85%	1 P:y	-5.339	0.67	40 C	
				1.75%	2 P:y	-5.563	1.00	5 P	
				1.48%	1 P:y	-5.339	0.67	38 C	
				1.39%	1 P:x	-5.339	0.67	36 C	
				1.22%	2 P:x	-5.563	1.00	5 P	
				1.16%	1 P:y	-5.339	0.67	7 C	
				1.11%	1 P:y	-5.339	0.67	33 C	
				1.10%	1 P:y	-5.339	0.67	30 C	
-11.913	2.00	266	A	30.51%	2 D:z2	-4.129	2.00	2 Pd	
				10.60%	2 D:yz	-4.129	2.00	2 Pd	
				6.69%	1 P:y	-5.339	0.67	16 C	
				6.04%	1 P:y	-5.339	0.67	13 C	
				4.82%	2 D:xy	-4.129	2.00	2 Pd	
				4.49%	2 D:xz	-4.129	2.00	2 Pd	
				2.28%	1 D:xy	-7.605	1.20	1 Fe	
				2.08%	1 P:y	-5.339	0.67	15 C	
				2.01%	1 P:y	-5.339	0.67	17 C	
				1.78%	2 P:y	-5.563	1.00	4 P	
				1.69%	1 P:x	-5.339	0.67	16 C	
				1.31%	1 P:x	-5.339	0.67	13 C	
				1.00%	1 P:z	-11.270	1.67	108 F	
-11.719	2.00	267	A	7.28%	1 P:y	-5.339	0.67	19 C	
				7.12%	1 P:y	-5.339	0.67	22 C	
				6.23%	1 P:z	-5.339	0.67	57 C	
				5.65%	1 P:z	-5.339	0.67	27 C	
				4.60%	2 D:yz	-4.129	2.00	2 Pd	
				4.09%	1 P:x	-5.339	0.67	22 C	
				4.00%	1 P:y	-5.339	0.67	13 C	
				3.96%	1 P:y	-5.339	0.67	16 C	
				3.50%	1 P:x	-5.339	0.67	27 C	
				2.98%	1 P:y	-5.339	0.67	21 C	
				2.31%	1 P:x	-5.339	0.67	26 C	
				2.16%	1 P:z	-5.339	0.67	26 C	
				2.02%	1 P:z	-5.339	0.67	19 C	
				1.89%	1 P:x	-5.339	0.67	21 C	
				1.89%	1 P:x	-5.339	0.67	19 C	
				1.42%	1 P:y	-5.339	0.67	23 C	
				1.37%	1 P:x	-5.339	0.67	28 C	
				1.35%	1 P:x	-5.339	0.67	23 C	

			1.33%	1 P:y	-5.339	0.67	15 C	
			1.21%	1 P:x	-5.339	0.67	57 C	
			1.12%	1 P:y	-5.339	0.67	57 C	
			1.10%	1 P:x	-5.339	0.67	13 C	
			1.09%	1 P:z	-5.339	0.67	22 C	
			1.07%	1 P:y	-5.339	0.67	18 C	
-11.652	2.00	268 A	18.61%	1 P:y	-5.339	0.67	14 C	
			16.59%	1 P:y	-5.339	0.67	17 C	
			14.77%	1 P:y	-5.339	0.67	18 C	
			12.78%	1 P:y	-5.339	0.67	15 C	
			4.55%	1 P:x	-5.339	0.67	14 C	
			4.05%	1 P:x	-5.339	0.67	17 C	
			3.62%	1 P:x	-5.339	0.67	18 C	
			3.22%	1 P:x	-5.339	0.67	15 C	
			1.29%	1 P:y	-5.339	0.67	51 C	
			1.07%	1 P:y	-5.339	0.67	48 C	
-11.586	2.00	269 A	17.29%	1 P:y	-5.339	0.67	44 C	
			15.91%	1 P:y	-5.339	0.67	41 C	
			7.25%	1 P:y	-5.339	0.67	43 C	
			5.34%	1 P:x	-5.339	0.67	44 C	
			4.76%	1 P:x	-5.339	0.67	41 C	
			4.26%	1 P:y	-5.339	0.67	45 C	
			2.87%	1 P:y	-5.339	0.67	46 C	
			2.32%	1 P:x	-5.339	0.67	43 C	
			1.33%	1 P:x	-5.339	0.67	45 C	
			1.28%	1 P:y	-5.339	0.67	24 C	
			1.27%	1 P:y	-5.339	0.67	34 C	
			1.23%	2 D:xz	-4.129	2.00	2 Pd	
			1.20%	1 P:z	-5.339	0.67	41 C	
			1.17%	1 P:y	-5.339	0.67	20 C	
			1.12%	1 P:z	-5.339	0.67	44 C	
			1.11%	1 P:y	-5.339	0.67	33 C	
			1.10%	1 P:y	-5.339	0.67	42 C	
			1.06%	1 P:y	-5.339	0.67	23 C	
			1.06%	1 P:x	-5.339	0.67	20 C	
-11.508	2.00	270 A	6.51%	1 P:y	-5.339	0.67	33 C	
			6.23%	1 P:y	-5.339	0.67	30 C	
			3.52%	1 P:y	-5.339	0.67	46 C	
			3.29%	1 P:y	-5.339	0.67	43 C	
			2.86%	1 P:y	-5.339	0.67	21 C	
			2.81%	1 P:y	-5.339	0.67	24 C	
			2.75%	1 P:y	-5.339	0.67	34 C	
			2.01%	1 P:x	-5.339	0.67	10 C	
			1.96%	1 P:z	-5.339	0.67	10 C	

			1.84%	2 D:xz	-4.129	2.00	2 Pd		
			1.80%	1 P:z	-5.339	0.67	7 C		
			1.73%	1 D:x2-y2	-7.605	1.20	1 Fe		
			1.73%	1 P:y	-5.339	0.67	32 C		
			1.71%	1 P:y	-5.339	0.67	7 C		
			1.66%	1 P:y	-5.339	0.67	42 C		
			1.63%	1 P:x	-5.339	0.67	21 C		
			1.58%	1 P:z	-5.339	0.67	30 C		
			1.55%	2 D:z2	-4.129	2.00	2 Pd		
			1.49%	1 P:x	-5.339	0.67	24 C		
			1.48%	1 P:z	-5.339	0.67	33 C		
			1.43%	1 P:y	-5.339	0.67	10 C		
			1.21%	1 P:z	-5.339	0.67	25 C		
			1.20%	1 P:y	-5.339	0.67	19 C		
			1.14%	1 P:y	-5.339	0.67	45 C		
			1.12%	2 D:x2-y2	-4.129	2.00	2 Pd		
			1.08%	1 P:z	-5.339	0.67	29 C		
			1.07%	2 P:x	-5.563	1.00	3 P		
			1.07%	1 P:x	-5.339	0.67	9 C		
			1.01%	1 P:x	-5.339	0.67	33 C		
			1.00%	1 P:x	-5.339	0.67	43 C		
-11.452	2.00	271 A	13.75%	1 P:y	-5.339	0.67	42 C		
			12.65%	1 P:y	-5.339	0.67	46 C		
			12.40%	1 P:y	-5.339	0.67	45 C		
			9.19%	1 P:y	-5.339	0.67	43 C		
			4.28%	1 P:x	-5.339	0.67	42 C		
			4.05%	1 P:x	-5.339	0.67	45 C		
			3.69%	1 P:x	-5.339	0.67	46 C		
			3.00%	1 P:x	-5.339	0.67	43 C		
			1.89%	1 P:y	-5.339	0.67	32 C		
			1.57%	1 P:y	-5.339	0.67	35 C		
			1.54%	1 P:y	-5.339	0.67	30 C		
			1.26%	1 P:y	-5.339	0.67	33 C		
			1.12%	1 D:x2-y2	-7.605	1.20	1 Fe		
-11.408	2.00	272 A	23.75%	1 P:y	-5.339	0.67	50 C		
			21.88%	1 P:y	-5.339	0.67	47 C		
			10.71%	1 P:y	-5.339	0.67	49 C		
			5.39%	1 P:y	-5.339	0.67	51 C		
			4.63%	1 P:y	-5.339	0.67	52 C		
			1.62%	2 D:z2	-4.129	2.00	2 Pd		
			1.61%	2 D:xz	-4.129	2.00	2 Pd		
			1.18%	1 P:y	-5.339	0.67	48 C		
			1.05%	1 P:x	-5.339	0.67	7 C		
			1.03%	1 D:yz	10.341	0.00	3 P		

-11.390	2.00	273	A	8.38%	1	P:y	-5.339	0.67	20 C
				7.44%	1	P:y	-5.339	0.67	24 C
				7.35%	1	P:y	-5.339	0.67	23 C
				5.91%	1	P:y	-5.339	0.67	21 C
				4.46%	1	P:x	-5.339	0.67	23 C
				4.16%	1	P:x	-5.339	0.67	20 C
				3.81%	1	P:x	-5.339	0.67	24 C
				3.44%	1	P:x	-5.339	0.67	21 C
				3.16%	1	P:y	-5.339	0.67	45 C
				2.64%	1	P:y	-5.339	0.67	42 C
				2.15%	1	P:z	-5.339	0.67	28 C
				1.91%	1	P:y	-5.339	0.67	44 C
				1.72%	1	P:z	-5.339	0.67	25 C
				1.71%	1	P:y	-5.339	0.67	41 C
				1.66%	1	P:x	-5.339	0.67	28 C
				1.57%	2	D:xz	-4.129	2.00	2 Pd
				1.48%	1	P:x	-5.339	0.67	25 C
				1.38%	2	D:z2	-4.129	2.00	2 Pd
				1.33%	1	P:y	-5.339	0.67	50 C
				1.22%	1	P:y	-5.339	0.67	47 C
				1.19%	1	P:z	-5.339	0.67	24 C
				1.18%	1	P:z	-5.339	0.67	57 C
				1.15%	1	P:y	-5.339	0.67	49 C
				1.00%	1	P:x	-5.339	0.67	45 C
-11.287	2.00	274	A	8.41%	1	P:y	-5.339	0.67	48 C
				7.58%	1	P:y	-5.339	0.67	51 C
				7.42%	1	P:z	-5.339	0.67	29 C
				7.30%	1	P:y	-5.339	0.67	52 C
				6.33%	1	P:z	-5.339	0.67	26 C
				5.47%	1	P:y	-5.339	0.67	49 C
				5.09%	1	P:z	-5.339	0.67	25 C
				4.85%	1	P:z	-5.339	0.67	28 C
				4.57%	1	P:x	-5.339	0.67	29 C
				4.46%	1	P:x	-5.339	0.67	26 C
				4.19%	1	P:x	-5.339	0.67	25 C
				3.50%	1	P:x	-5.339	0.67	28 C
				1.43%	1	P:y	-5.339	0.67	21 C
				1.32%	1	P:y	-5.339	0.67	24 C
				1.22%	1	P:y	-5.339	0.67	35 C
				1.22%	1	P:y	-5.339	0.67	31 C
				1.15%	1	P:y	-5.339	0.67	32 C
				1.04%	1	P:x	-5.339	0.67	12 C
-11.238	2.00	275	A	8.93%	1	P:y	-5.339	0.67	35 C
				8.50%	1	P:y	-5.339	0.67	32 C

			6.65%	1 P:y	-5.339	0.67	31 C	
			4.94%	1 P:y	-5.339	0.67	34 C	
			3.79%	1 P:z	-5.339	0.67	27 C	
			3.48%	1 P:z	-5.339	0.67	57 C	
			3.27%	1 P:z	-5.339	0.67	28 C	
			3.20%	1 P:y	-5.339	0.67	23 C	
			2.86%	1 P:z	-5.339	0.67	25 C	
			2.82%	1 P:y	-5.339	0.67	20 C	
			2.53%	1 P:x	-5.339	0.67	27 C	
			2.44%	1 P:x	-5.339	0.67	57 C	
			2.15%	1 P:x	-5.339	0.67	28 C	
			2.11%	1 P:z	-5.339	0.67	35 C	
			2.07%	1 P:x	-5.339	0.67	25 C	
			1.93%	1 P:z	-5.339	0.67	31 C	
			1.78%	2 D:xz	-4.129	2.00	2 Pd	
			1.68%	1 P:z	-5.339	0.67	32 C	
			1.55%	1 P:x	-5.339	0.67	35 C	
			1.46%	1 P:x	-5.339	0.67	32 C	
			1.39%	1 P:x	-5.339	0.67	23 C	
			1.30%	1 P:z	-5.339	0.67	34 C	
			1.28%	1 P:x	-5.339	0.67	20 C	
			1.17%	1 P:x	-5.339	0.67	19 C	
			1.17%	1 P:y	-5.339	0.67	45 C	
			1.11%	1 P:y	-5.339	0.67	42 C	
-11.230	2.00	276 A	14.51%	1 P:y	-5.339	0.67	48 C	
			13.89%	1 P:y	-5.339	0.67	51 C	
			9.98%	1 P:y	-5.339	0.67	52 C	
			7.33%	1 P:y	-5.339	0.67	49 C	
			4.28%	1 P:z	-5.339	0.67	29 C	
			3.34%	1 P:z	-5.339	0.67	26 C	
			2.83%	1 P:z	-5.339	0.67	28 C	
			2.64%	1 P:z	-5.339	0.67	25 C	
			2.39%	1 P:x	-5.339	0.67	26 C	
			2.34%	1 P:x	-5.339	0.67	29 C	
			2.16%	1 P:x	-5.339	0.67	25 C	
			2.11%	1 P:x	-5.339	0.67	28 C	
			2.00%	1 P:y	-5.339	0.67	15 C	
			1.65%	1 P:y	-5.339	0.67	18 C	
			1.25%	1 P:y	-5.339	0.67	14 C	
			1.06%	1 P:y	-5.339	0.67	35 C	
			1.06%	1 P:y	-5.339	0.67	32 C	
-11.183	2.00	277 A	7.93%	1 P:y	-5.339	0.67	31 C	
			7.83%	1 P:y	-5.339	0.67	34 C	
			4.52%	1 P:z	-5.339	0.67	27 C	

			4.40%	1 P:z	-5.339	0.67	57 C	
			4.22%	1 P:y	-5.339	0.67	35 C	
			3.65%	1 P:y	-5.339	0.67	32 C	
			3.23%	1 P:x	-5.339	0.67	27 C	
			3.17%	1 P:z	-5.339	0.67	26 C	
			3.03%	1 P:x	-5.339	0.67	57 C	
			2.99%	1 P:x	-5.339	0.67	19 C	
			2.85%	1 P:z	-5.339	0.67	29 C	
			2.16%	2 D:z2	-4.129	2.00	2 Pd	
			1.94%	1 P:x	-5.339	0.67	26 C	
			1.93%	1 P:z	-5.339	0.67	31 C	
			1.92%	1 P:z	-5.339	0.67	34 C	
			1.75%	1 P:x	-5.339	0.67	29 C	
			1.70%	1 P:y	-5.339	0.67	22 C	
			1.59%	2 D:xz	-4.129	2.00	2 Pd	
			1.48%	1 P:y	-5.339	0.67	16 C	
			1.48%	1 P:y	-5.339	0.67	13 C	
			1.38%	1 P:y	-5.339	0.67	19 C	
			1.29%	1 P:x	-5.339	0.67	34 C	
			1.15%	1 P:x	-5.339	0.67	31 C	
			1.13%	1 P:z	-5.339	0.67	35 C	
			1.06%	1 P:x	-5.339	0.67	22 C	
			1.04%	2 P:y	-5.563	1.00	4 P	
			1.02%	5 S	-3.388	0.00	2 Pd	
-11.115	2.00	278 A	8.43%	2 D:z2	-4.129	2.00	2 Pd	
			6.07%	5 S	-3.388	0.00	2 Pd	
			4.98%	2 D:xz	-4.129	2.00	2 Pd	
			4.44%	1 P:y	-5.339	0.67	33 C	
			3.90%	1 P:y	-5.339	0.67	19 C	
			3.44%	1 P:y	-5.339	0.67	22 C	
			3.44%	1 P:y	-5.339	0.67	30 C	
			2.71%	1 P:y	-5.339	0.67	32 C	
			2.60%	1 P:y	-5.339	0.67	16 C	
			2.38%	1 P:x	-5.339	0.67	57 C	
			2.18%	1 P:y	-5.339	0.67	13 C	
			2.14%	1 P:y	-5.339	0.67	35 C	
			2.09%	1 P:x	-5.339	0.67	22 C	
			1.95%	2 P:y	-5.563	1.00	4 P	
			1.53%	1 P:z	-5.339	0.67	27 C	
			1.29%	1 P:z	-5.339	0.67	28 C	
			1.22%	2 D:x2-y2	-4.129	2.00	2 Pd	
			1.18%	1 P:y	-5.339	0.67	20 C	
			1.15%	1 P:z	-5.339	0.67	25 C	
			1.10%	1 P:y	-5.339	0.67	18 C	

			1.03%	6 S	1.008	0.00	2 Pd		
-11.091	2.00	279 A	8.99%	1 P:z	-5.339	0.67	8 C		
			8.79%	1 P:x	-5.339	0.67	8 C		
			8.27%	1 P:x	-5.339	0.67	11 C		
			7.26%	1 P:z	-5.339	0.67	11 C		
			7.21%	1 P:x	-5.339	0.67	12 C		
			6.56%	1 P:z	-5.339	0.67	12 C		
			6.07%	1 P:x	-5.339	0.67	9 C		
			5.88%	1 P:y	-5.339	0.67	8 C		
			5.71%	1 P:z	-5.339	0.67	9 C		
			5.65%	1 P:y	-5.339	0.67	11 C		
			5.16%	1 P:y	-5.339	0.67	12 C		
			3.92%	1 P:y	-5.339	0.67	9 C		
			2.58%	1 P:y	-5.339	0.67	49 C		
			2.48%	1 P:y	-5.339	0.67	52 C		
			1.61%	1 P:y	-5.339	0.67	48 C		
			1.54%	1 P:y	-5.339	0.67	51 C		
-10.873	2.00	280 A	5.46%	1 P:x	-5.339	0.67	7 C		
			4.89%	1 D:x2-y2	-7.605	1.20	1 Fe		
			4.59%	1 P:x	-5.339	0.67	10 C		
			4.27%	1 P:y	-5.339	0.67	33 C		
			4.00%	1 P:z	-5.339	0.67	10 C		
			3.90%	1 P:y	-5.339	0.67	30 C		
			3.48%	1 P:z	-5.339	0.67	7 C		
			3.04%	1 P:y	-5.339	0.67	10 C		
			2.05%	1 P:y	-5.339	0.67	7 C		
			1.82%	1 P:y	-5.339	0.67	47 C		
			1.81%	2 P:x	-5.563	1.00	3 P		
			1.79%	2 P:y	-5.563	1.00	5 P		
			1.72%	1 P:z	-5.339	0.67	9 C		
			1.56%	1 P:y	-5.339	0.67	34 C		
			1.54%	1 P:y	-5.339	0.67	31 C		
			1.52%	1 P:x	-5.339	0.67	9 C		
			1.47%	1 P:z	-5.339	0.67	12 C		
			1.40%	3 S	-14.037	2.00	3 P		
			1.38%	4 P:x	0.627	0.00	2 Pd		
			1.35%	1 P:y	-5.339	0.67	41 C		
			1.34%	1 D:yz	-7.605	1.20	1 Fe		
			1.33%	2 P:x	-5.563	1.00	5 P		
			1.33%	1 P:y	-5.339	0.67	50 C		
			1.29%	1 P:y	-5.339	0.67	9 C		
			1.22%	3 S	-14.037	2.00	5 P		
			1.20%	1 P:x	-5.339	0.67	12 C		
			1.19%	1 D:xy	-7.605	1.20	1 Fe		

			1.18%	1 P:y	-5.339	0.67	12 C		
			1.14%	4 P:y	0.627	0.00	2 Pd		
			1.00%	1 D:xz	-7.605	1.20	1 Fe		
-10.813	2.00	281 A	34.65%	1 D:x2-y2	-7.605	1.20	1 Fe		
			16.14%	1 D:xy	-7.605	1.20	1 Fe		
			3.58%	1 D:xz	-7.605	1.20	1 Fe		
			2.16%	5 S	-3.388	0.00	2 Pd		
			2.09%	4 P:y	0.627	0.00	2 Pd		
			1.93%	2 P:y	-5.563	1.00	4 P		
			1.70%	1 P:y	-5.339	0.67	6 C		
			1.68%	1 P:y	-5.339	0.67	7 C		
			1.49%	4 S	-5.371	2.00	1 Fe		
			1.43%	1 P:x	-5.339	0.67	10 C		
			1.41%	1 P:z	-5.339	0.67	7 C		
			1.28%	1 P:z	-5.339	0.67	10 C		
			1.20%	2 D:xz	-4.129	2.00	2 Pd		
			1.02%	1 P:x	-5.339	0.67	36 C		
-10.371	2.00	282 A	65.70%	1 D:z2	-7.605	1.20	1 Fe		
			16.06%	1 D:xz	-7.605	1.20	1 Fe		
			2.17%	1 P:x	-5.339	0.67	40 C		
			1.85%	4 S	-5.371	2.00	1 Fe		
			1.84%	1 P:x	-5.339	0.67	56 C		
			1.62%	1 P:x	-5.339	0.67	55 C		
			1.23%	1 P:x	-5.339	0.67	39 C		
			1.20%	1 D:yz	-7.605	1.20	1 Fe		
-10.288	2.00	283 A	65.54%	1 D:yz	-7.605	1.20	1 Fe		
			4.97%	1 D:xz	-7.605	1.20	1 Fe		
			3.26%	1 D:xy	-7.605	1.20	1 Fe		
			2.90%	1 D:x2-y2	-7.605	1.20	1 Fe		
			2.67%	1 P:x	-5.339	0.67	6 C		
			2.52%	1 P:x	-5.339	0.67	37 C		
			2.50%	1 P:x	-5.339	0.67	53 C		
			2.07%	1 P:x	-5.339	0.67	36 C		
			1.37%	2 D:yz	-4.129	2.00	2 Pd		
-8.851	0.00	284 A	13.35%	2 D:x2-y2	-4.129	2.00	2 Pd		
			11.02%	2 P:y	-5.563	1.00	4 P		
			6.96%	2 D:xy	-4.129	2.00	2 Pd		
			5.61%	2 P:x	-5.563	1.00	3 P		
			5.42%	1 D:x2-y2	-7.605	1.20	1 Fe		
			5.23%	2 P:y	-5.563	1.00	5 P		
			4.46%	3 S	-14.037	2.00	4 P		
			3.66%	3 S	-14.037	2.00	5 P		
			3.47%	3 S	-14.037	2.00	3 P		
			3.39%	1 D:xy	-7.605	1.20	1 Fe		

			2.81%	2 D:xz	-4.129	2.00	2 Pd	
			2.75%	2 P:x	-5.563	1.00	5 P	
			1.83%	1 P:x	-5.339	0.67	53 C	
			1.73%	1 D:z2	-7.605	1.20	1 Fe	
			-1.42%	3 D:x2-y2	5.439	0.00	2 Pd	
			1.31%	1 P:x	-5.339	0.67	37 C	
			-1.24%	3 P:y	2.157	0.00	4 P	
			-1.18%	4 S	3.043	0.00	4 P	
			1.12%	2 P:x	-5.563	1.00	4 P	
			1.10%	1 P:x	-5.339	0.67	6 C	
			1.01%	1 P:y	-5.339	0.67	16 C	
			1.00%	5 S	-3.388	0.00	2 Pd	
-7.988	0.00	285 A	30.38%	1 D:xy	-7.605	1.20	1 Fe	
			16.29%	1 D:x2-y2	-7.605	1.20	1 Fe	
			8.49%	1 P:x	-5.339	0.67	55 C	
			6.18%	1 P:x	-5.339	0.67	39 C	
			6.08%	1 P:x	-5.339	0.67	36 C	
			4.24%	1 P:x	-5.339	0.67	6 C	
			4.20%	1 D:yz	-7.605	1.20	1 Fe	
			3.70%	1 P:x	-5.339	0.67	53 C	
			2.27%	1 P:x	-5.339	0.67	38 C	
			1.94%	1 P:y	-5.339	0.67	39 C	
			1.10%	1 P:x	-5.339	0.67	37 C	
			1.05%	4 P:z	0.627	0.00	2 Pd	

All SINGLET-SINGLET excitation energies

Table S7 Excitation energies E in a.u. and eV, dE wrt prev. cycle, oscillator strengths f in a.u.

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.34205E-02	0.93078E-01	0.39803E-03	0.11E-09
2	0.54821E-02	0.14918	0.11535E-02	0.38E-10
3	0.91162E-02	0.24806	0.12345E-02	0.13E-09
4	0.19013E-01	0.51737	0.59088E-03	0.17E-09
5	0.25399E-01	0.69113	0.14681E-02	0.41E-09
6	0.25602E-01	0.69665	0.22019E-02	0.10E-08
7	0.29259E-01	0.79619	0.53408E-03	0.53E-10
8	0.30594E-01	0.83250	0.41459E-01	0.80E-07
9	0.31043E-01	0.84473	0.19143E-01	0.67E-08
10	0.32122E-01	0.87408	0.63049E-02	0.20E-07

Table S8 Transition dipole moments mu (x,y,z) in a.u. (weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	0.93078E-01	0.39803E-03	0.21804	-0.31923	-0.15843
2	0.14918	0.11535E-02	0.12733	0.21987	-0.50105
3	0.24806	0.12345E-02	0.28964	0.23676	0.25137
4	0.51737	0.59088E-03	0.89151E-01	-0.17285E-01	0.19588
5	0.69113	0.14681E-02	-0.18489	0.12165	0.19421
6	0.69665	0.22019E-02	0.17092	-0.30685	-0.75131E-01
7	0.79619	0.53408E-03	0.12513	-0.10746	0.13262E-01
8	0.83250	0.41459E-01	-0.21483	0.84902	-1.1250
9	0.84473	0.19143E-01	-0.22688	0.50043	-0.78937
10	0.87408	0.63049E-02	0.32479	0.11652	-0.41875

Table S9 Major MO -> MO transitions for the above excitations

Excitation Nr.	Occupied to virtual orbitals	Contribution weight (sum=1)	contribibutions to transition dipole moment x	y	z
1: 282a	-> 284a	0.9303	0.2451	-0.7024	0.1809
1: 283a	-> 284a	0.0694	0.1586	0.1646	-0.4259
2: 283a	-> 284a	0.9214	0.4565	0.4738	-1.2262
2: 282a	-> 284a	0.0686	-0.0526	0.1507	-0.0388
2: 276a	-> 284a	0.0046	-0.1150	-0.1756	0.2016
2: 278a	-> 284a	0.0045	-0.1101	-0.0757	0.1386
3: 281a	-> 284a	0.9985	0.5196	0.3953	0.4383
4: 280a	-> 284a	0.7875	0.7574	-0.6632	1.4375
4: 279a	-> 284a	0.2107	-0.5805	0.6851	-1.1590
5: 278a	-> 284a	0.7405	-0.6578	-0.4523	0.8281
5: 276a	-> 284a	0.2029	0.3558	0.5431	-0.6235
5: 277a	-> 284a	0.0542	-0.0813	0.0875	0.0883
5: 283a	-> 284a	0.0008	-0.0062	-0.0064	0.0166
6: 277a	-> 284a	0.9366	0.3368	-0.3625	-0.3655
6: 278a	-> 284a	0.0436	-0.1589	-0.1093	0.2001
6: 276a	-> 284a	0.0101	0.0791	0.1208	-0.1387
6: 279a	-> 284a	0.0064	0.0874	-0.1031	0.1744
6: 275a	-> 284a	0.0015	-0.0100	0.0014	0.0016
7: 275a	-> 284a	0.9915	0.2411	-0.0346	-0.0378
7: 272a	-> 284a	0.0019	-0.0433	-0.0359	-0.0321
7: 276a	-> 284a	0.0015	-0.0288	-0.0440	0.0505
7: 277a	-> 284a	0.0014	0.0122	-0.0132	-0.0133
7: 274a	-> 284a	0.0011	0.0015	0.0038	0.0118

7: 273a	-> 284a	0.0009	-0.0022	-0.0023	-0.0081
8: 279a	-> 284a	0.4787	-0.6898	0.8140	-1.3772
8: 273a	-> 284a	0.2979	0.0379	0.0405	0.1402
8: 280a	-> 284a	0.1189	-0.2320	0.2031	-0.4403
8: 276a	-> 284a	0.0715	0.1925	0.2938	-0.3373
8: 278a	-> 284a	0.0129	0.0791	0.0544	-0.0996
8: 277a	-> 284a	0.0043	0.0208	-0.0224	-0.0226
8: 269a	-> 284a	0.0030	0.0991	-0.0294	0.0509
8: 275a	-> 284a	0.0028	0.0125	-0.0018	-0.0020
8: 283a	-> 284a	0.0014	0.0076	0.0079	-0.0204
8: 264a	-> 284a	0.0008	0.0145	-0.0362	0.0172
8: 254a	-> 284a	0.0007	0.0093	0.0044	0.0202
8: 272a	-> 284a	0.0006	0.0233	0.0193	0.0173
8: 268a	-> 284a	0.0004	-0.0063	-0.0028	-0.0058
8: 270a	-> 284a	0.0004	0.0063	0.0068	0.0069
8: 265a	-> 284a	0.0003	0.0662	-0.0115	-0.0135
8: 279a	-> 286a	0.0003	0.0053	-0.0020	0.0083
8: 279a	-> 285a	0.0003	-0.0008	-0.0008	0.0082
8: 279a	-> 292a	0.0003	0.0149	-0.0103	0.0200
8: 253a	-> 284a	0.0003	-0.0176	-0.0602	0.0019
8: 279a	-> 291a	0.0002	-0.0069	-0.0117	0.0059
9: 273a	-> 284a	0.6798	-0.0569	-0.0608	-0.2102
9: 279a	-> 284a	0.2249	-0.4693	0.5538	-0.9370
9: 280a	-> 284a	0.0596	-0.1631	0.1428	-0.3096
9: 272a	-> 284a	0.0101	0.0966	0.0802	0.0717
9: 274a	-> 284a	0.0096	-0.0043	-0.0110	-0.0337
9: 276a	-> 284a	0.0056	0.0537	0.0820	-0.0941
9: 277a	-> 284a	0.0023	0.0150	-0.0162	-0.0163
9: 270a	-> 284a	0.0020	0.0140	0.0150	0.0153
9: 278a	-> 284a	0.0010	0.0217	0.0149	-0.0273
9: 269a	-> 284a	0.0009	0.0539	-0.0160	0.0277
9: 254a	-> 284a	0.0004	0.0071	0.0033	0.0154
9: 283a	-> 284a	0.0004	0.0040	0.0042	-0.0108
9: 268a	-> 284a	0.0003	-0.0050	-0.0022	-0.0046
9: 265a	-> 284a	0.0002	0.0529	-0.0092	-0.0108
9: 279a	-> 292a	0.0002	0.0117	-0.0081	0.0157
9: 279a	-> 286a	0.0002	0.0039	-0.0015	0.0060
9: 264a	-> 284a	0.0002	0.0066	-0.0166	0.0079
9: 279a	-> 285a	0.0002	-0.0006	-0.0006	0.0059
9: 279a	-> 296a	0.0001	-0.0056	-0.0042	0.0213

9: 279a -> 300a 0.0001 -0.0066 -0.0015 0.0275

10: 274a -> 284a 0.6816 -0.0354 -0.0909 -0.2790
10: 276a -> 284a 0.2079 0.3203 0.4889 -0.5613
10: 278a -> 284a 0.0453 0.1447 0.0995 -0.1822
10: 279a -> 284a 0.0270 0.1599 -0.1886 0.3191
10: 272a -> 284a 0.0163 -0.1205 -0.1000 -0.0894
10: 280a -> 284a 0.0105 0.0674 -0.0590 0.1279
10: 283a -> 284a 0.0022 0.0092 0.0096 -0.0248
10: 275a -> 284a 0.0014 0.0086 -0.0012 -0.0014
10: 271a -> 284a 0.0013 -0.0021 -0.0016 -0.0004
10: 270a -> 284a 0.0011 -0.0100 -0.0108 -0.0109
10: 268a -> 284a 0.0005 0.0064 0.0028 0.0059
10: 265a -> 284a 0.0005 -0.0758 0.0132 0.0155
10: 269a -> 284a 0.0003 0.0317 -0.0094 0.0163
10: 267a -> 284a 0.0003 -0.0009 -0.0082 0.0015
10: 274a -> 288a 0.0003 0.0007 0.0033 0.0100
10: 254a -> 284a 0.0002 -0.0046 -0.0022 -0.0099
10: 282a -> 284a 0.0002 -0.0011 0.0031 -0.0008
10: 264a -> 284a 0.0002 0.0065 -0.0163 0.0077
10: 261a -> 284a 0.0002 -0.0052 -0.0137 0.0037
10: 276a -> 288a 0.0001 -0.0054 -0.0032 0.0162

Table S10 All SINGLET-TRIPLET excitation energies

no.	E/a.u.	E/eV	f	Symmetry
1:	0.00184	0.05013	0.000	A
2:	0.00275	0.07470	0.000	A
3:	0.00811	0.22063	0.000	A
4:	0.01563	0.42533	0.000	A
5:	0.01941	0.52804	0.000	A
6:	0.02327	0.63311	0.000	A
7:	0.02498	0.67964	0.000	A
8:	0.02547	0.69304	0.000	A
9:	0.02903	0.78994	0.000	A
10:	0.02924	0.79564	0.000	A

II. Computational details for $[Pd(dppf)(PPh_3)][BF_4]_2$

Table S11 Optimized coordinates

1.Fe	2.611956	7.694644	3.527565
2.Pd	3.519712	10.555322	3.589468
3.P	1.355615	10.640181	2.555293
4.P	4.199086	12.779425	3.622805
5.P	5.441151	9.407477	4.309934
6.C	1.011482	9.054786	3.347634
7.C	-0.098831	11.692931	2.862916
8.C	-1.038204	11.364700	3.852034
9.H	-0.929381	10.454905	4.440473
10.C	-2.143613	12.188907	4.060634
11.H	-2.881764	11.918251	4.814262
12.C	-2.314137	13.341878	3.291159
13.H	-3.183458	13.978084	3.449806
14.C	-1.377438	13.671914	2.306775
15.H	-1.516770	14.563192	1.697695
16.C	-0.269531	12.855346	2.092596
17.H	0.443867	13.103320	1.307839
18.C	4.506586	13.257084	1.893698
19.C	3.607742	14.060858	1.176541
20.H	2.736151	14.483782	1.672967
21.C	3.839006	14.330047	-0.173508
22.H	3.145982	14.965393	-0.722246
23.C	4.956329	13.793256	-0.817184
24.H	5.135501	14.011547	-1.869250
25.C	5.847203	12.981024	-0.108966
26.H	6.724028	12.567038	-0.605400
27.C	5.624671	12.705758	1.238367
28.H	6.324850	12.073520	1.782856
29.C	5.719103	13.155615	4.575698
30.C	5.759465	12.749667	5.920581
31.H	4.942638	12.168343	6.344278
32.C	6.833443	13.111018	6.729574
33.H	6.852726	12.801710	7.773034
34.C	7.876328	13.880463	6.203601
35.H	8.713111	14.168528	6.838254
36.C	7.834926	14.294083	4.871148
37.H	8.636277	14.906819	4.462467
38.C	6.759744	13.937757	4.054356
39.H	6.731941	14.281549	3.023064
40.C	1.962922	13.380679	5.203554
41.H	1.858700	12.302237	5.325214

42.C	1.115963	14.245928	5.895447
43.H	0.349212	13.844080	6.555165
44.C	1.255055	15.626584	5.740254
45.H	0.595045	16.303842	6.280540
46.C	2.245359	16.142128	4.898506
47.H	2.360266	17.218946	4.784175
48.C	3.104490	15.283657	4.216170
49.H	3.892804	15.695217	3.590187
50.C	7.091574	9.638513	3.570775
51.C	8.054738	10.388924	4.265323
52.H	7.835995	10.786211	5.254676
53.C	9.307382	10.609252	3.694875
54.H	10.054202	11.176220	4.247721
55.C	9.604992	10.103133	2.428092
56.H	10.586424	10.273769	1.988749
57.C	8.646348	9.363437	1.731138
58.H	8.880617	8.947846	0.752789
59.C	7.394258	9.129424	2.295832
60.H	6.673743	8.524190	1.751482
61.C	4.728954	7.916733	3.585110
62.C	4.251091	7.807890	2.214096
63.H	4.379923	8.541153	1.427840
64.C	3.616745	6.547258	2.071688
65.H	3.164160	6.163767	1.163135
66.C	3.659019	5.885869	3.340716
67.H	3.249984	4.904962	3.557989
68.C	4.332141	6.725966	4.275951
69.H	4.523063	6.504050	5.320946
70.C	5.658615	9.022318	6.074095
71.C	4.650992	9.381423	6.984014
72.H	3.781068	9.936277	6.634672
73.C	4.765818	9.032171	8.327886
74.H	3.985511	9.314622	9.033123
75.C	5.889609	8.329098	8.770764
76.H	5.983417	8.061447	9.822059
77.C	6.894923	7.970857	7.867928
78.H	7.769581	7.421937	8.212245
79.C	6.785108	8.315795	6.521049
80.H	7.570019	8.034837	5.821570
81.C	1.357812	10.303691	0.766330
82.C	2.568692	10.272131	0.059594
83.H	3.498703	10.528865	0.566839
84.C	2.577549	9.942886	-1.295334
85.H	3.518184	9.927156	-1.843901

86.C	1.378845	9.652431	-1.951040
87.H	1.385312	9.398607	-3.009814
88.C	0.167518	9.703352	-1.254583
89.H	-0.768142	9.491131	-1.768784
90.C	0.150475	10.035004	0.098979
91.H	-0.796463	10.086946	0.634323
92.C	1.296648	8.799714	4.753908
93.H	1.556156	9.547812	5.494958
94.C	1.110697	7.415007	4.997500
95.H	1.246604	6.909834	5.947996
96.C	0.727482	6.800553	3.762854
97.H	0.518716	5.745122	3.620291
98.C	0.667036	7.802653	2.747119
99.H	0.418774	7.645182	1.702703
100.C	2.956568	13.892505	4.358196

Table S12 Selected individual LMO bond orders greater than 0.002 in magnitude, with the overlap between the hybrids in the NLMO given:

Atom I	Atom J	NLMO	Bond Order	Hybrid Overlap
1	2	95	0.0081389	0.0347257
1	2	97	0.0983318	0.1219075
1	2	102	-0.0045498	-0.0024346
1	2	104	-0.0058678	-0.0119854
1	2	105	0.0020799	0.0882473
1	2	106	0.0020523	0.0039109
1	2	116	0.0123444	0.1645879
1	2	189	0.0144842	0.1591485
1	2	191	0.0021685	0.0780583
1	2	227	0.0025902	0.0950380
1	2	234	0.0021565	0.0145666
1	2	235	-0.0478824	-0.0488385

Table S13 Natural localized molecular orbital (NLMO) analysis for NLMOs with a bond order greater than 0.02:

Hybridization/Polarization Analysis of NLMOs in NAO Basis:

NLMO/Occupancy/Percent from Parent NBO/ Atomic Hybrid Contributions

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97. (2.00000) 82.4330% LP (3)Fe 1
82.564% Fe 1 s(0.47%)p 0.03(0.01%)d99.99(99.52%)
4.917% Pd 2 s(8.84%)p 0.08(0.69%)d10.23(90.47%)
0.695% P 3 s(15.42%)p 5.24(80.76%)d 0.25(3.81%)
3.234% P 4 s(34.01%)p 1.94(65.99%)d 0.00(0.00%)
0.755% P 5 s(6.64%)p13.32(88.43%)d 0.74(4.93%)
0.414% C 6 s(1.34%)p71.03(95.50%)d 2.34(3.15%)
0.114% C 7 s(35.02%)p 1.84(64.37%)d 0.02(0.62%)
0.062% C 13 s(10.28%)p 8.70(89.38%)d 0.03(0.34%)
0.032% C 14 s(4.18%)p22.86(95.61%)d 0.05(0.20%)
0.021% C 16 s(0.28%)p99.99(99.70%)d 0.07(0.02%)
0.026% C 18 s(2.27%)p42.95(97.36%)d 0.16(0.37%)
0.053% C 19 s(20.42%)p 3.87(78.93%)d 0.03(0.65%)
0.021% C 20 s(14.91%)p 5.68(84.77%)d 0.02(0.31%)
0.012% C 22 s(1.05%)p94.55(98.92%)d 0.03(0.03%)
0.026% C 24 s(15.23%)p 5.53(84.18%)d 0.04(0.59%)
0.011% C 25 s(49.00%)p 1.04(50.78%)d 0.00(0.22%)
0.017% C 29 s(39.43%)p 1.50(59.31%)d 0.03(1.26%)
0.088% C 30 s(33.13%)p 1.99(66.04%)d 0.02(0.83%)
0.771% C 36 s(0.57%)p99.99(97.63%)d 3.15(1.80%)
0.042% C 37 s(17.47%)p 3.47(60.56%)d 1.26(21.97%)
0.236% C 38 s(0.30%)p99.99(96.91%)d 9.21(2.79%)
1.002% C 39 s(6.27%)p14.90(93.41%)d 0.05(0.32%)
1.599% C 40 s(0.90%)p99.99(98.96%)d 0.15(0.13%)
0.014% C 41 s(15.46%)p 5.27(81.47%)d 0.20(3.06%)
0.015% C 47 s(38.08%)p 1.57(59.70%)d 0.06(2.22%)
0.043% C 53 s(9.74%)p 6.92(67.43%)d 2.34(22.83%)
0.452% C 54 s(0.71%)p99.99(98.10%)d 1.67(1.19%)
1.766% C 55 s(4.94%)p19.21(94.96%)d 0.02(0.10%)
0.821% C 56 s(0.70%)p99.99(98.87%)d 0.61(0.43%)
0.032% C 57 s(28.14%)p 2.50(70.22%)d 0.06(1.65%)
0.011% H 83 s(94.13%)p 0.06(5.87%)
0.018% H 97 s(93.46%)p 0.07(6.54%)

Table S14 List of selected MOs, ordered by energy, with the most significant SFO gross populations

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-12.274	2.00	212 A	13.51%	2 D:yz	-4.129	2.00	2 Pd
			10.07%	2 D:xz	-4.129	2.00	2 Pd
			9.52%	1 P:x	-5.339	0.67	53 C
			8.72%	1 D:xy	-7.605	1.20	1 Fe
			7.19%	1 P:x	-5.339	0.67	55 C
			4.60%	1 P:x	-5.339	0.67	56 C
			3.27%	1 P:x	-5.339	0.67	37 C
			2.41%	1 D:x2-y2	-7.605	1.20	1 Fe
			1.79%	2 D:z2	-4.129	2.00	2 Pd
			1.71%	2 P:x	-5.563	1.00	3 P
			1.50%	1 P:x	-5.339	0.67	39 C
			1.41%	1 D:yz	-7.605	1.20	1 Fe
			1.35%	1 P:x	-5.339	0.67	6 C
			1.32%	3 P:z	-0.725	0.00	1 Fe
			1.27%	2 P:y	-5.563	1.00	5 P
			1.19%	1 P:y	-5.339	0.67	55 C
			1.16%	1 P:y	-5.339	0.67	40 C
			1.09%	1 P:x	-5.339	0.67	40 C
-12.152	2.00	213 A	14.52%	2 D:yz	-4.129	2.00	2 Pd
			10.26%	2 D:xz	-4.129	2.00	2 Pd
			9.23%	1 P:x	-5.339	0.67	39 C
			6.22%	1 P:x	-5.339	0.67	55 C
			6.19%	1 P:x	-5.339	0.67	37 C
			4.90%	1 P:x	-5.339	0.67	6 C
			3.99%	1 P:x	-5.339	0.67	36 C
			3.06%	3 P:y	-0.725	0.00	1 Fe
			2.62%	1 D:x2-y2	-7.605	1.20	1 Fe
			2.11%	2 D:z2	-4.129	2.00	2 Pd
			2.05%	1 P:y	-5.339	0.67	39 C
			1.89%	2 P:y	-5.563	1.00	4 P
			1.65%	1 P:x	-5.339	0.67	53 C
			1.65%	1 P:x	-5.339	0.67	54 C
			1.58%	1 P:x	-5.339	0.67	40 C
			1.29%	1 P:z	-5.339	0.67	13 C
			1.20%	1 P:y	-5.339	0.67	37 C
			1.15%	1 D:xz	-7.605	1.20	1 Fe
			1.07%	1 P:y	-5.339	0.67	6 C
			1.02%	2 D:x2-y2	-4.129	2.00	2 Pd
-12.039	2.00	214 A	17.23%	2 D:x2-y2	-4.129	2.00	2 Pd

				10.67%	2	D:yz	-4.129	2.00	2 Pd
				9.26%	2	D:z2	-4.129	2.00	2 Pd
				3.64%	2	D:xz	-4.129	2.00	2 Pd
				3.47%	1	P:x	-5.339	0.67	55 C
				3.43%	2	D:xy	-4.129	2.00	2 Pd
				2.66%	1	P:x	-5.339	0.67	6 C
				1.64%	1	P:x	-5.339	0.67	19 C
				1.55%	1	P:x	-5.339	0.67	30 C
				1.41%	1	P:x	-5.339	0.67	53 C
				1.36%	3	P:y	-0.725	0.00	1 Fe
				1.35%	2	P:x	-5.563	1.00	3 P
				1.33%	1	P:x	-5.339	0.67	39 C
				1.29%	2	P:x	-5.563	1.00	5 P
				1.20%	1	P:z	-5.339	0.67	47 C
				1.08%	1	P:x	-5.339	0.67	36 C
				1.04%	1	P:z	-5.339	0.67	30 C
-11.960	2.00	215	A	27.31%	2	D:xy	-4.129	2.00	2 Pd
				13.92%	2	D:z2	-4.129	2.00	2 Pd
				9.70%	2	D:xz	-4.129	2.00	2 Pd
				4.13%	1	P:x	-5.339	0.67	38 C
				3.26%	1	P:x	-5.339	0.67	36 C
				2.22%	1	P:x	-5.339	0.67	40 C
				2.21%	1	P:y	-5.339	0.67	36 C
				1.89%	1	P:x	-5.339	0.67	56 C
				1.32%	1	P:x	-5.339	0.67	54 C
				1.29%	1	P:x	-5.339	0.67	39 C
				1.12%	3	P:z	-0.725	0.00	1 Fe
				1.11%	1	P:z	-5.339	0.67	41 C
				1.04%	1	D:x2-y2	-7.605	1.20	1 Fe
-11.792	2.00	216	A	16.42%	2	D:yz	-4.129	2.00	2 Pd
				9.28%	2	D:xz	-4.129	2.00	2 Pd
				6.84%	2	D:x2-y2	-4.129	2.00	2 Pd
				4.23%	1	D:xy	-7.605	1.20	1 Fe
				3.85%	2	D:xy	-4.129	2.00	2 Pd
				3.51%	1	D:x2-y2	-7.605	1.20	1 Fe
				3.46%	2	D:z2	-4.129	2.00	2 Pd
				3.21%	2	P:y	-5.563	1.00	5 P
				2.82%	2	P:x	-5.563	1.00	3 P
				1.89%	1	P:x	-5.339	0.67	6 C
				1.57%	1	P:x	-5.339	0.67	36 C
				1.43%	1	P:z	-5.339	0.67	13 C
				1.29%	1	P:y	-5.339	0.67	44 C
				1.26%	1	P:y	-5.339	0.67	7 C
				1.09%	1	P:x	-5.339	0.67	39 C

-11.701	2.00	217 A	14.89%	2 D:yz	-4.129	2.00	2 Pd		
			9.01%	1 P:x	-5.339	0.67	56 C		
			8.44%	1 P:x	-5.339	0.67	54 C		
			6.62%	1 P:x	-5.339	0.67	40 C		
			5.53%	1 P:x	-5.339	0.67	38 C		
			4.34%	2 D:xy	-4.129	2.00	2 Pd		
			3.86%	3 P:z	-0.725	0.00	1 Fe		
			3.34%	1 P:x	-5.339	0.67	37 C		
			3.05%	1 P:x	-5.339	0.67	53 C		
			2.41%	1 P:y	-5.339	0.67	40 C		
			2.22%	1 P:x	-5.339	0.67	6 C		
			1.82%	2 D:z2	-4.129	2.00	2 Pd		
			1.80%	1 D:yz	-7.605	1.20	1 Fe		
			1.39%	2 P:x	-5.563	1.00	3 P		
			1.18%	1 P:y	-5.339	0.67	38 C		
			1.15%	1 P:y	-5.339	0.67	37 C		
			1.01%	1 P:x	-5.339	0.67	39 C		
-11.517	2.00	218 A	34.52%	2 D:z2	-4.129	2.00	2 Pd		
			10.60%	2 D:xz	-4.129	2.00	2 Pd		
			5.23%	1 P:y	-5.339	0.67	16 C		
			4.12%	1 P:y	-5.339	0.67	13 C		
			3.74%	2 D:yz	-4.129	2.00	2 Pd		
			2.81%	2 D:xy	-4.129	2.00	2 Pd		
			2.75%	2 P:y	-5.563	1.00	4 P		
			2.33%	1 P:y	-5.339	0.67	15 C		
			2.20%	1 P:x	-5.339	0.67	16 C		
			1.73%	1 P:y	-5.339	0.67	17 C		
			1.71%	1 P:x	-5.339	0.67	13 C		
			1.33%	1 P:z	-5.339	0.67	13 C		
			1.32%	5 S	-3.388	0.00	2 Pd		
			1.22%	1 P:y	-5.339	0.67	22 C		
			1.03%	1 P:y	-5.339	0.67	19 C		
-11.337	2.00	219 A	18.97%	1 P:y	-5.339	0.67	44 C		
			17.91%	1 P:y	-5.339	0.67	41 C		
			9.26%	1 P:y	-5.339	0.67	43 C		
			5.60%	1 P:x	-5.339	0.67	44 C		
			5.06%	1 P:x	-5.339	0.67	41 C		
			4.51%	1 P:y	-5.339	0.67	46 C		
			3.52%	1 P:y	-5.339	0.67	45 C		
			2.80%	1 P:x	-5.339	0.67	43 C		
			2.22%	1 P:y	-5.339	0.67	34 C		
			2.14%	1 P:y	-5.339	0.67	33 C		
			1.59%	1 P:y	-5.339	0.67	31 C		
			1.58%	1 P:y	-5.339	0.67	30 C		

			1.29%	2 D:xz	-4.129	2.00	2 Pd		
			1.08%	1 P:x	-5.339	0.67	46 C		
			1.05%	1 P:x	-5.339	0.67	45 C		
-11.238	2.00	220 A	5.24%	1 P:y	-5.339	0.67	50 C		
			4.66%	1 P:y	-5.339	0.67	47 C		
			4.33%	1 P:y	-5.339	0.67	49 C		
			4.04%	1 P:z	-5.339	0.67	10 C		
			3.64%	1 P:y	-5.339	0.67	13 C		
			3.40%	1 P:y	-5.339	0.67	16 C		
			3.29%	1 P:z	-5.339	0.67	7 C		
			2.46%	1 P:y	-5.339	0.67	52 C		
			2.39%	1 P:y	-5.339	0.67	10 C		
			2.15%	1 P:z	-5.339	0.67	9 C		
			2.15%	1 P:x	-5.339	0.67	10 C		
			2.14%	1 P:z	-5.339	0.67	27 C		
			2.05%	1 P:z	-5.339	0.67	57 C		
			2.02%	1 P:y	-5.339	0.67	45 C		
			2.00%	1 P:y	-5.339	0.67	7 C		
			1.97%	1 P:y	-5.339	0.67	42 C		
			1.87%	1 P:x	-5.339	0.67	7 C		
			1.64%	1 P:x	-5.339	0.67	13 C		
			1.60%	2 D:yz	-4.129	2.00	2 Pd		
			1.48%	1 P:y	-5.339	0.67	17 C		
			1.45%	1 P:x	-5.339	0.67	16 C		
			1.36%	1 P:y	-5.339	0.67	33 C		
			1.36%	1 P:x	-5.339	0.67	27 C		
			1.34%	1 P:y	-5.339	0.67	9 C		
			1.30%	1 P:y	-5.339	0.67	22 C		
			1.25%	1 P:x	-5.339	0.67	9 C		
			1.17%	1 P:y	-5.339	0.67	30 C		
			1.11%	1 P:x	-5.339	0.67	28 C		
			1.04%	1 P:y	-5.339	0.67	19 C		
			1.03%	2 D:xy	-4.129	2.00	2 Pd		
			1.03%	1 P:y	-5.339	0.67	46 C		
-11.213	2.00	221 A	16.34%	1 P:y	-5.339	0.67	42 C		
			15.43%	1 P:y	-5.339	0.67	45 C		
			13.61%	1 P:y	-5.339	0.67	46 C		
			9.97%	1 P:y	-5.339	0.67	43 C		
			4.91%	1 P:x	-5.339	0.67	42 C		
			4.72%	1 P:x	-5.339	0.67	45 C		
			3.72%	1 P:x	-5.339	0.67	46 C		
			3.22%	1 P:y	-5.339	0.67	50 C		
			2.97%	1 P:x	-5.339	0.67	43 C		
			2.93%	1 P:y	-5.339	0.67	47 C		

			1.10%	1 P:y	-5.339	0.67	49 C		
			1.03%	1 P:y	-5.339	0.67	51 C		
-11.182	2.00	222 A	7.42%	1 P:y	-5.339	0.67	22 C		
			6.76%	1 P:y	-5.339	0.67	19 C		
			5.15%	1 P:y	-5.339	0.67	30 C		
			5.15%	1 P:y	-5.339	0.67	33 C		
			3.90%	1 P:y	-5.339	0.67	21 C		
			3.80%	1 P:y	-5.339	0.67	32 C		
			3.52%	1 P:z	-5.339	0.67	57 C		
			3.11%	1 D:x2-y2	-7.605	1.20	1 Fe		
			2.46%	1 P:x	-5.339	0.67	22 C		
			2.38%	1 P:y	-5.339	0.67	35 C		
			2.20%	1 P:z	-5.339	0.67	27 C		
			1.78%	1 P:y	-5.339	0.67	18 C		
			1.64%	1 P:x	-5.339	0.67	27 C		
			1.59%	1 P:y	-5.339	0.67	14 C		
			1.56%	2 D:x2-y2	-4.129	2.00	2 Pd		
			1.55%	1 P:y	-5.339	0.67	24 C		
			1.53%	1 P:x	-5.339	0.67	21 C		
			1.38%	1 P:x	-5.339	0.67	26 C		
			1.37%	1 P:z	-5.339	0.67	19 C		
			1.36%	1 P:y	-5.339	0.67	23 C		
			1.33%	1 P:x	-5.339	0.67	19 C		
			1.33%	1 P:z	-5.339	0.67	26 C		
			1.31%	1 P:y	-5.339	0.67	15 C		
			1.30%	1 P:z	-5.339	0.67	30 C		
			1.22%	1 P:z	-5.339	0.67	33 C		
			1.16%	1 D:xy	-7.605	1.20	1 Fe		
			1.06%	2 P:x	-5.563	1.00	3 P		
			1.03%	1 P:z	-5.339	0.67	10 C		
-11.150	2.00	223 A	15.67%	1 P:y	-5.339	0.67	50 C		
			14.63%	1 P:y	-5.339	0.67	47 C		
			6.55%	1 P:y	-5.339	0.67	51 C		
			3.61%	1 P:y	-5.339	0.67	49 C		
			3.19%	1 P:y	-5.339	0.67	48 C		
			2.91%	1 P:y	-5.339	0.67	15 C		
			2.67%	1 P:y	-5.339	0.67	18 C		
			2.28%	1 P:y	-5.339	0.67	33 C		
			2.19%	1 P:y	-5.339	0.67	30 C		
			1.51%	1 P:y	-5.339	0.67	13 C		
			1.29%	1 P:y	-5.339	0.67	16 C		
			1.26%	1 P:x	-5.339	0.67	15 C		
			1.21%	1 P:y	-5.339	0.67	46 C		
			1.14%	1 P:y	-5.339	0.67	43 C		

			1.10%	1 P:y	-5.339	0.67	22 C
			1.06%	1 P:y	-5.339	0.67	52 C
			1.03%	1 P:y	-5.339	0.67	19 C
-11.107	2.00	224 A	11.68%	1 P:y	-5.339	0.67	17 C
			11.67%	1 P:y	-5.339	0.67	14 C
			7.51%	1 P:y	-5.339	0.67	18 C
			5.97%	1 P:y	-5.339	0.67	15 C
			5.63%	1 P:x	-5.339	0.67	14 C
			4.86%	1 P:x	-5.339	0.67	17 C
			3.97%	1 P:y	-5.339	0.67	49 C
			3.88%	1 P:x	-5.339	0.67	18 C
			3.81%	1 P:y	-5.339	0.67	52 C
			2.57%	1 P:x	-5.339	0.67	15 C
			1.50%	1 P:y	-5.339	0.67	47 C
			1.45%	1 P:y	-5.339	0.67	50 C
			1.36%	1 P:z	-5.339	0.67	17 C
			1.28%	1 P:z	-5.339	0.67	14 C
			1.22%	1 P:y	-5.339	0.67	48 C
			1.19%	1 P:z	-5.339	0.67	27 C
			1.17%	1 P:z	-5.339	0.67	57 C
-11.023	2.00	225 A	18.40%	1 P:y	-5.339	0.67	48 C
			17.44%	1 P:y	-5.339	0.67	51 C
			15.26%	1 P:y	-5.339	0.67	52 C
			11.88%	1 P:y	-5.339	0.67	49 C
			2.29%	1 P:y	-5.339	0.67	31 C
			2.16%	1 P:y	-5.339	0.67	34 C
			1.47%	1 P:y	-5.339	0.67	35 C
			1.25%	1 P:y	-5.339	0.67	32 C
			1.14%	1 P:z	-5.339	0.67	51 C
			1.08%	1 P:z	-5.339	0.67	48 C
-10.994	2.00	226 A	10.94%	1 P:y	-5.339	0.67	35 C
			10.71%	1 P:y	-5.339	0.67	32 C
			10.30%	1 P:y	-5.339	0.67	31 C
			8.70%	1 P:y	-5.339	0.67	34 C
			3.12%	1 P:z	-5.339	0.67	35 C
			2.54%	1 P:z	-5.339	0.67	32 C
			2.50%	1 P:y	-5.339	0.67	14 C
			2.44%	1 P:z	-5.339	0.67	31 C
			2.22%	1 P:z	-5.339	0.67	34 C
			2.19%	1 P:y	-5.339	0.67	51 C
			2.14%	1 P:y	-5.339	0.67	17 C
			2.07%	1 P:y	-5.339	0.67	48 C
			2.01%	1 P:x	-5.339	0.67	35 C
			1.74%	1 P:x	-5.339	0.67	32 C

			1.72%	1 P:x	-5.339	0.67	31 C		
			1.55%	1 P:x	-5.339	0.67	34 C		
			1.51%	1 P:y	-5.339	0.67	20 C		
			1.48%	1 P:y	-5.339	0.67	52 C		
			1.47%	1 P:y	-5.339	0.67	15 C		
			1.46%	1 P:y	-5.339	0.67	18 C		
			1.42%	1 P:y	-5.339	0.67	21 C		
			1.18%	1 P:y	-5.339	0.67	49 C		
			1.15%	1 P:y	-5.339	0.67	24 C		
			1.10%	1 P:x	-5.339	0.67	14 C		
-10.882	2.00	227 A	8.33%	1 P:y	-5.339	0.67	24 C		
			6.67%	1 P:y	-5.339	0.67	21 C		
			5.75%	1 P:z	-5.339	0.67	28 C		
			5.61%	1 P:z	-5.339	0.67	25 C		
			5.57%	1 P:y	-5.339	0.67	20 C		
			4.49%	1 P:x	-5.339	0.67	28 C		
			4.34%	1 P:y	-5.339	0.67	23 C		
			4.01%	1 P:x	-5.339	0.67	25 C		
			2.29%	1 P:z	-5.339	0.67	29 C		
			2.27%	1 P:x	-5.339	0.67	24 C		
			2.19%	1 P:y	-5.339	0.67	35 C		
			2.17%	1 P:x	-5.339	0.67	21 C		
			2.05%	1 P:y	-5.339	0.67	32 C		
			2.03%	1 P:y	-5.339	0.67	31 C		
			1.97%	1 P:z	-5.339	0.67	57 C		
			1.91%	1 P:z	-5.339	0.67	27 C		
			1.90%	1 P:x	-5.339	0.67	23 C		
			1.82%	1 P:y	-5.339	0.67	34 C		
			1.82%	1 P:x	-5.339	0.67	20 C		
			1.51%	1 P:y	-5.339	0.67	16 C		
			1.47%	2 D:xz	-4.129	2.00	2 Pd		
			1.30%	1 P:x	-5.339	0.67	29 C		
			1.27%	1 P:x	-5.339	0.67	27 C		
			1.11%	1 P:y	-5.339	0.67	13 C		
			1.08%	2 D:z2	-4.129	2.00	2 Pd		
-10.840	2.00	228 A	11.35%	1 P:z	-5.339	0.67	8 C		
			9.91%	1 P:z	-5.339	0.67	11 C		
			8.34%	1 P:z	-5.339	0.67	12 C		
			6.87%	1 P:z	-5.339	0.67	9 C		
			6.36%	1 P:y	-5.339	0.67	11 C		
			6.21%	1 P:y	-5.339	0.67	8 C		
			6.20%	1 P:x	-5.339	0.67	8 C		
			6.10%	1 P:x	-5.339	0.67	11 C		
			5.42%	1 P:y	-5.339	0.67	12 C		

				5.30%	1 P:x	-5.339	0.67	12 C	
				4.17%	1 P:x	-5.339	0.67	9 C	
				3.99%	1 P:y	-5.339	0.67	9 C	
				1.91%	1 P:y	-5.339	0.67	49 C	
				1.78%	1 P:y	-5.339	0.67	52 C	
-10.801	2.00	229	A	6.63%	1 P:y	-5.339	0.67	20 C	
				6.47%	1 P:y	-5.339	0.67	23 C	
				6.23%	1 P:y	-5.339	0.67	21 C	
				6.05%	1 P:y	-5.339	0.67	24 C	
				4.38%	2 D:xz	-4.129	2.00	2 Pd	
				3.66%	1 P:z	-5.339	0.67	28 C	
				3.35%	1 P:z	-5.339	0.67	25 C	
				3.20%	5 S	-3.388	0.00	2 Pd	
				3.10%	1 P:x	-5.339	0.67	24 C	
				2.89%	2 D:z2	-4.129	2.00	2 Pd	
				2.63%	1 P:x	-5.339	0.67	28 C	
				2.36%	1 P:x	-5.339	0.67	25 C	
				2.36%	1 P:x	-5.339	0.67	21 C	
				2.21%	1 P:z	-5.339	0.67	57 C	
				2.17%	1 P:y	-5.339	0.67	15 C	
				1.96%	1 P:y	-5.339	0.67	16 C	
				1.82%	1 P:x	-5.339	0.67	20 C	
				1.82%	1 P:z	-5.339	0.67	27 C	
				1.81%	1 P:y	-5.339	0.67	13 C	
				1.76%	1 P:y	-5.339	0.67	18 C	
				1.72%	1 P:x	-5.339	0.67	23 C	
				1.39%	1 P:y	-5.339	0.67	33 C	
				1.38%	1 P:x	-5.339	0.67	27 C	
				1.17%	1 P:x	-5.339	0.67	18 C	
				1.08%	1 P:y	-5.339	0.67	35 C	
				1.06%	1 P:z	-5.339	0.67	24 C	
				1.03%	1 P:y	-5.339	0.67	32 C	
-10.743	2.00	230	A	7.92%	1 P:z	-5.339	0.67	29 C	
				6.95%	1 P:z	-5.339	0.67	26 C	
				5.94%	1 P:z	-5.339	0.67	25 C	
				5.58%	1 P:z	-5.339	0.67	28 C	
				4.77%	1 P:x	-5.339	0.67	29 C	
				4.59%	2 D:z2	-4.129	2.00	2 Pd	
				4.48%	1 P:x	-5.339	0.67	26 C	
				4.33%	1 P:x	-5.339	0.67	25 C	
				3.92%	5 S	-3.388	0.00	2 Pd	
				3.87%	1 P:x	-5.339	0.67	28 C	
				2.89%	1 P:y	-5.339	0.67	33 C	
				2.68%	2 D:xz	-4.129	2.00	2 Pd	

				2.64%	1 P:y	-5.339	0.67	30 C	
				1.59%	1 P:y	-5.339	0.67	16 C	
				1.57%	1 P:y	-5.339	0.67	13 C	
				1.35%	1 P:y	-5.339	0.67	34 C	
				1.29%	1 P:y	-5.339	0.67	31 C	
				1.10%	1 D:x2-y2	-7.605	1.20	1 Fe	
-10.653	2.00	231	A	6.92%	1 P:z	-5.339	0.67	27 C	
				6.45%	1 P:y	-5.339	0.67	22 C	
				6.27%	1 P:z	-5.339	0.67	26 C	
				6.22%	1 P:z	-5.339	0.67	57 C	
				6.10%	1 P:x	-5.339	0.67	57 C	
				5.59%	1 P:y	-5.339	0.67	19 C	
				5.49%	1 P:z	-5.339	0.67	29 C	
				5.17%	1 P:x	-5.339	0.67	27 C	
				4.11%	1 P:x	-5.339	0.67	26 C	
				3.41%	1 P:y	-5.339	0.67	23 C	
				3.39%	1 P:x	-5.339	0.67	19 C	
				3.30%	1 P:x	-5.339	0.67	29 C	
				3.24%	1 D:x2-y2	-7.605	1.20	1 Fe	
				3.15%	1 P:y	-5.339	0.67	20 C	
				2.32%	1 P:x	-5.339	0.67	22 C	
				1.27%	2 D:z2	-4.129	2.00	2 Pd	
				1.25%	1 D:xy	-7.605	1.20	1 Fe	
				1.22%	5 S	-3.388	0.00	2 Pd	
-10.588	2.00	232	A	6.93%	1 P:z	-5.339	0.67	10 C	
				6.26%	1 P:z	-5.339	0.67	7 C	
				5.03%	1 P:x	-5.339	0.67	7 C	
				4.31%	1 P:y	-5.339	0.67	10 C	
				4.22%	1 P:x	-5.339	0.67	10 C	
				3.28%	1 P:y	-5.339	0.67	7 C	
				3.24%	1 P:z	-5.339	0.67	9 C	
				3.02%	1 P:z	-5.339	0.67	12 C	
				2.81%	1 P:y	-5.339	0.67	47 C	
				2.40%	2 P:x	-5.563	1.00	3 P	
				2.02%	5 S	-3.388	0.00	2 Pd	
				2.01%	1 P:y	-5.339	0.67	9 C	
				1.91%	1 P:y	-5.339	0.67	33 C	
				1.89%	1 P:y	-5.339	0.67	50 C	
				1.83%	4 P:x	0.627	0.00	2 Pd	
				1.77%	2 D:xz	-4.129	2.00	2 Pd	
				1.72%	1 P:y	-5.339	0.67	12 C	
				1.67%	3 S	-14.037	2.00	3 P	
				1.60%	1 P:y	-5.339	0.67	30 C	
				1.58%	1 P:x	-5.339	0.67	9 C	

			1.50%	1 P:x	-5.339	0.67	12 C	
			1.44%	1 P:y	-5.339	0.67	49 C	
			1.26%	1 P:y	-5.339	0.67	52 C	
			1.20%	1 D:yz	-7.605	1.20	1 Fe	
			1.02%	2 P:y	-5.563	1.00	5 P	
-10.454	2.00	233 A	35.48%	1 D:x2-y2	-7.605	1.20	1 Fe	
			16.70%	1 D:xy	-7.605	1.20	1 Fe	
			3.18%	1 D:xz	-7.605	1.20	1 Fe	
			2.89%	2 P:y	-5.563	1.00	4 P	
			2.84%	4 P:y	0.627	0.00	2 Pd	
			2.80%	1 P:y	-5.339	0.67	19 C	
			2.27%	1 P:y	-5.339	0.67	22 C	
			1.89%	4 S	-5.371	2.00	1 Fe	
			1.64%	1 P:y	-5.339	0.67	16 C	
			1.57%	1 P:y	-5.339	0.67	13 C	
			1.46%	3 S	-14.037	2.00	4 P	
			1.33%	1 P:x	-5.339	0.67	36 C	
-10.061	2.00	234 A	66.53%	1 D:z2	-7.605	1.20	1 Fe	
			15.74%	1 D:xz	-7.605	1.20	1 Fe	
			2.34%	1 P:x	-5.339	0.67	40 C	
			1.89%	1 P:x	-5.339	0.67	56 C	
			1.71%	4 S	-5.371	2.00	1 Fe	
			1.57%	1 P:x	-5.339	0.67	55 C	
			1.24%	1 P:x	-5.339	0.67	39 C	
-9.982	2.00	235 A	66.74%	1 D:yz	-7.605	1.20	1 Fe	
			3.98%	1 D:xz	-7.605	1.20	1 Fe	
			3.28%	1 D:xy	-7.605	1.20	1 Fe	
			2.50%	1 P:x	-5.339	0.67	6 C	
			2.50%	1 P:x	-5.339	0.67	37 C	
			2.47%	1 P:x	-5.339	0.67	53 C	
			2.07%	1 P:x	-5.339	0.67	36 C	
			1.61%	1 D:x2-y2	-7.605	1.20	1 Fe	
			1.57%	1 D:z2	-7.605	1.20	1 Fe	
			1.36%	2 D:yz	-4.129	2.00	2 Pd	
-8.508	0.00	236 A	13.57%	2 D:x2-y2	-4.129	2.00	2 Pd	
			12.13%	2 P:y	-5.563	1.00	4 P	
			6.80%	2 D:xy	-4.129	2.00	2 Pd	
			5.36%	2 P:y	-5.563	1.00	5 P	
			5.29%	2 P:x	-5.563	1.00	3 P	
			4.57%	3 S	-14.037	2.00	4 P	
			4.40%	1 D:x2-y2	-7.605	1.20	1 Fe	
			3.75%	1 D:xy	-7.605	1.20	1 Fe	
			3.63%	3 S	-14.037	2.00	5 P	
			3.46%	3 S	-14.037	2.00	3 P	

			2.86%	2 D:xz	-4.129	2.00	2 Pd	
			2.76%	2 P:x	-5.563	1.00	5 P	
			1.77%	1 P:x	-5.339	0.67	53 C	
			1.65%	1 D:z2	-7.605	1.20	1 Fe	
			-1.47%	3 D:x2-y2	5.439	0.00	2 Pd	
			1.22%	1 P:x	-5.339	0.67	37 C	
			-1.09%	4 S	3.043	0.00	4 P	
			1.00%	1 P:x	-5.339	0.67	6 C	
-7.658	0.00	237 A	29.60%	1 D:xy	-7.605	1.20	1 Fe	
			18.41%	1 D:x2-y2	-7.605	1.20	1 Fe	
			8.33%	1 P:x	-5.339	0.67	55 C	
			6.44%	1 P:x	-5.339	0.67	36 C	
			6.06%	1 P:x	-5.339	0.67	39 C	
			3.89%	1 P:x	-5.339	0.67	6 C	
			3.88%	1 P:x	-5.339	0.67	53 C	
			3.54%	1 D:yz	-7.605	1.20	1 Fe	
			2.52%	1 P:x	-5.339	0.67	38 C	
			1.90%	1 P:y	-5.339	0.67	39 C	
			1.16%	1 P:y	-5.339	0.67	36 C	
			1.11%	1 P:x	-5.339	0.67	56 C	

Table S15 Excitation energies E in a.u. and eV, dE wrt prev. cycle, oscillator strengths f in a.u.

no.	E/a.u.	E/eV	f	dE/a.u.	
1	0.31710E-01	0.86288	0.23258E-02	0.65E-09	
2	0.37660E-01	1.0248	0.34653E-01	0.43E-08	
3	0.49116E-01	1.3365	0.52517E-01	0.45E-08	
4	0.54131E-01	1.4730	0.14607E-01	0.21E-08	
5	0.55696E-01	1.5156	0.45631E-02	0.37E-08	
6	0.58125E-01	1.5817	0.36737E-02	0.10E-07	
7	0.58815E-01	1.6004	0.14777E-01	0.64E-08	
8	0.60668E-01	1.6508	0.60768E-02	0.24E-08	
9	0.61495E-01	1.6734	0.37403E-01	0.74E-08	
10	0.63869E-01	1.7380	0.25371E-02	0.32E-06	

Table S16 Transition dipole moments mu (x,y,z) in a.u. (weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	0.86288	0.23258E-02	0.17584	-0.76630E-01	0.27060
2	1.0248	0.34653E-01	0.60988	-0.54417	0.84388
3	1.3365	0.52517E-01	1.2430	0.15422E-01	0.24203
4	1.4730	0.14607E-01	0.60989	0.11084	-0.14324
5	1.5156	0.45631E-02	0.27184	-0.15367	-0.15932
6	1.5817	0.36737E-02	-0.65243E-01	0.15420	-0.25840
7	1.6004	0.14777E-01	0.41607	-0.44156	0.93750E-01
8	1.6508	0.60768E-02	-0.63291E-01	-0.27084	0.26997
9	1.6734	0.37403E-01	-0.61254	0.71108	-0.17754
10	1.7380	0.25371E-02	-0.11516	0.19356	-0.94119E-01

Table S17 Major MO -> MO transitions for the above excitations

Excitation Nr.	Occupied to virtual orbitals		Contribution weight (sum=1)	contribibutions to transition dipole moment x	y	z
1:	217a	-> 218a	0.5839	0.9496	-0.6561	1.1571
1:	216a	-> 218a	0.4153	-0.6096	0.4926	-0.7352
2:	216a	-> 218a	0.5760	0.6588	-0.5323	0.7945
2:	217a	-> 218a	0.4061	0.7266	-0.5021	0.8854
2:	215a	-> 218a	0.0055	-0.2261	0.0156	0.0071
2:	213a	-> 218a	0.0033	-0.0632	0.0833	-0.0116
2:	216a	-> 219a	0.0017	-0.0118	-0.0023	-0.0225
2:	214a	-> 218a	0.0010	0.0122	0.0659	-0.0462
2:	200a	-> 218a	0.0005	-0.0103	0.0030	-0.0178
2:	217a	-> 222a	0.0004	-0.0245	0.0137	-0.0234
2:	211a	-> 218a	0.0004	-0.0075	-0.0047	0.0118
2:	209a	-> 218a	0.0004	-0.0328	-0.0141	0.0143
2:	216a	-> 222a	0.0003	-0.0108	0.0051	-0.0197
2:	210a	-> 218a	0.0002	-0.0119	-0.0230	0.0061
2:	216a	-> 225a	0.0002	0.0053	0.0055	-0.0200
2:	216a	-> 223a	0.0002	0.0018	0.0109	-0.0165
2:	212a	-> 218a	0.0002	0.0051	-0.0059	-0.0021
2:	217a	-> 233a	0.0001	-0.0118	0.0129	-0.0221
2:	217a	-> 225a	0.0001	-0.0106	0.0072	-0.0076
2:	197a	-> 218a	0.0001	-0.0070	0.0030	-0.0017
2:	216a	-> 228a	0.0001	0.0062	-0.0022	-0.0191
2:	199a	-> 218a	0.0001	-0.0010	0.0150	-0.0027
3:	215a	-> 218a	0.8828	2.5053	-0.1723	-0.0782
3:	213a	-> 218a	0.0651	-0.2467	0.3250	-0.0454
3:	214a	-> 218a	0.0324	-0.0594	-0.3216	0.2252
3:	211a	-> 218a	0.0032	-0.0195	-0.0122	0.0307
3:	216a	-> 218a	0.0024	0.0374	-0.0302	0.0451
3:	212a	-> 218a	0.0015	-0.0137	0.0158	0.0055
3:	204a	-> 218a	0.0013	0.0030	0.0167	0.0024
3:	217a	-> 218a	0.0012	0.0353	-0.0244	0.0430
3:	208a	-> 218a	0.0011	-0.0106	0.0214	0.0075

3: 215a	-> 222a	0.0009	-0.0763	0.0274	-0.0122
3: 209a	-> 218a	0.0008	-0.0441	-0.0189	0.0192
3: 206a	-> 218a	0.0008	-0.0104	0.0005	0.0044
3: 207a	-> 218a	0.0007	0.0102	0.0069	-0.0124
3: 198a	-> 218a	0.0004	-0.0099	0.0064	-0.0040
3: 205a	-> 218a	0.0004	0.0002	0.0003	-0.0043
3: 190a	-> 218a	0.0003	-0.0172	-0.0106	-0.0169
3: 217a	-> 219a	0.0002	-0.0011	0.0000	0.0016
3: 215a	-> 221a	0.0002	-0.0105	0.0056	0.0035
3: 215a	-> 229a	0.0001	-0.0061	0.0187	-0.0115
3: 213a	-> 220a	0.0001	-0.0028	0.0016	-0.0022

4: 214a	-> 218a	0.4422	0.2088	1.1313	-0.7922
4: 213a	-> 218a	0.4068	0.5874	-0.7740	0.1082
4: 215a	-> 218a	0.0750	0.6954	-0.0478	-0.0217
4: 211a	-> 218a	0.0338	-0.0608	-0.0379	0.0955
4: 209a	-> 218a	0.0165	-0.1878	-0.0804	0.0819
4: 210a	-> 218a	0.0106	-0.0649	-0.1256	0.0335
4: 212a	-> 218a	0.0090	-0.0323	0.0373	0.0129
4: 206a	-> 218a	0.0013	-0.0126	0.0006	0.0054
4: 204a	-> 218a	0.0005	0.0017	0.0096	0.0014
4: 216a	-> 218a	0.0004	0.0152	-0.0123	0.0184
4: 217a	-> 218a	0.0004	0.0187	-0.0129	0.0228
4: 208a	-> 218a	0.0002	-0.0046	0.0093	0.0033
4: 214a	-> 221a	0.0002	-0.0161	-0.0136	0.0241
4: 215a	-> 222a	0.0002	-0.0335	0.0120	-0.0054
4: 217a	-> 219a	0.0002	-0.0009	0.0000	0.0014
4: 213a	-> 222a	0.0001	-0.0196	0.0001	0.0123
4: 215a	-> 221a	0.0001	-0.0079	0.0042	0.0026
4: 198a	-> 218a	0.0001	-0.0048	0.0031	-0.0019
4: 213a	-> 229a	0.0001	-0.0050	-0.0001	0.0094
4: 201a	-> 218a	0.0001	-0.0071	-0.0102	-0.0033

5: 212a	-> 218a	0.9747	0.3304	-0.3816	-0.1320
5: 214a	-> 218a	0.0113	0.0329	0.1784	-0.1249
5: 210a	-> 218a	0.0036	0.0374	0.0723	-0.0193
5: 215a	-> 218a	0.0033	0.1446	-0.0099	-0.0045
5: 208a	-> 218a	0.0024	-0.0146	0.0295	0.0103
5: 207a	-> 218a	0.0011	0.0120	0.0082	-0.0146
5: 205a	-> 218a	0.0007	0.0003	0.0004	-0.0055
5: 203a	-> 218a	0.0007	-0.0245	-0.0502	-0.0278
5: 211a	-> 218a	0.0006	-0.0078	-0.0048	0.0122

6: 211a	-> 218a	0.4249	0.2080	0.1297	-0.3267
6: 210a	-> 218a	0.3973	-0.3830	-0.7413	0.1976
6: 214a	-> 218a	0.1025	0.0970	0.5256	-0.3680
6: 213a	-> 218a	0.0624	-0.2220	0.2926	-0.0409
6: 209a	-> 218a	0.0041	0.0903	0.0387	-0.0394
6: 204a	-> 218a	0.0017	0.0032	0.0177	0.0025
6: 205a	-> 218a	0.0015	0.0004	0.0005	-0.0076
6: 215a	-> 218a	0.0012	0.0846	-0.0058	-0.0026
6: 207a	-> 218a	0.0012	0.0122	0.0083	-0.0149
6: 208a	-> 218a	0.0005	0.0064	-0.0129	-0.0045
6: 212a	-> 218a	0.0003	0.0059	-0.0069	-0.0024
6: 217a	-> 218a	0.0002	-0.0123	0.0085	-0.0150
6: 199a	-> 218a	0.0002	0.0011	-0.0159	0.0029
6: 217a	-> 219a	0.0001	-0.0008	0.0000	0.0012

7: 211a	-> 218a	0.4737	0.2183	0.1361	-0.3430
7: 213a	-> 218a	0.2342	0.4275	-0.5633	0.0787
7: 210a	-> 218a	0.1141	0.2040	0.3949	-0.1052
7: 214a	-> 218a	0.0938	-0.0922	-0.4998	0.3500
7: 209a	-> 218a	0.0448	-0.2972	-0.1272	0.1296
7: 215a	-> 218a	0.0113	0.2595	-0.0178	-0.0081
7: 207a	-> 218a	0.0076	-0.0309	-0.0210	0.0377
7: 206a	-> 218a	0.0052	-0.0242	0.0011	0.0104
7: 205a	-> 218a	0.0042	-0.0006	-0.0008	0.0128
7: 208a	-> 218a	0.0023	0.0139	-0.0281	-0.0098
7: 217a	-> 218a	0.0017	0.0373	-0.0258	0.0454
7: 216a	-> 218a	0.0017	0.0283	-0.0228	0.0341
7: 212a	-> 218a	0.0006	0.0083	-0.0095	-0.0033
7: 203a	-> 218a	0.0005	0.0208	0.0427	0.0236
7: 204a	-> 218a	0.0004	-0.0014	-0.0081	-0.0011
7: 215a	-> 219a	0.0004	-0.0023	0.0071	-0.0029
7: 217a	-> 219a	0.0002	0.0010	0.0000	-0.0014
7: 199a	-> 218a	0.0002	-0.0012	0.0172	-0.0032
7: 215a	-> 222a	0.0002	-0.0333	0.0119	-0.0053
7: 192a	-> 218a	0.0002	-0.0010	0.0118	0.0025

8: 208a	-> 218a	0.7581	-0.2482	0.5012	0.1753
8: 210a	-> 218a	0.0710	-0.1584	-0.3066	0.0817
8: 214a	-> 218a	0.0686	-0.0777	-0.4208	0.2947
8: 213a	-> 218a	0.0570	0.2076	-0.2736	0.0382

8: 209a	-> 218a	0.0179	0.1848	0.0791	-0.0806
8: 206a	-> 218a	0.0121	0.0362	-0.0016	-0.0156
8: 207a	-> 218a	0.0071	0.0294	0.0200	-0.0359
8: 204a	-> 218a	0.0021	0.0034	0.0189	0.0027
8: 205a	-> 218a	0.0018	0.0004	0.0005	-0.0083
8: 211a	-> 218a	0.0007	-0.0083	-0.0052	0.0130
8: 217a	-> 219a	0.0004	0.0014	0.0000	-0.0020
8: 215a	-> 218a	0.0003	-0.0381	0.0026	0.0012
8: 216a	-> 218a	0.0002	0.0099	-0.0080	0.0120
8: 203a	-> 218a	0.0002	0.0132	0.0271	0.0150
8: 217a	-> 218a	0.0002	0.0121	-0.0084	0.0148
8: 210a	-> 221a	0.0001	0.0027	-0.0012	-0.0035
8: 192a	-> 218a	0.0001	-0.0008	0.0094	0.0020
8: 215a	-> 221a	0.0001	0.0067	-0.0036	-0.0022
8: 196a	-> 218a	0.0001	0.0028	0.0025	-0.0004
8: 197a	-> 218a	0.0001	-0.0043	0.0019	-0.0011

9: 209a	-> 218a	0.4741	-0.9454	-0.4047	0.4124
9: 207a	-> 218a	0.1451	0.1322	0.0898	-0.1612
9: 208a	-> 218a	0.1077	-0.0929	0.1876	0.0656
9: 213a	-> 218a	0.0992	-0.2721	0.3585	-0.0501
9: 210a	-> 218a	0.0611	0.1460	0.2825	-0.0753
9: 214a	-> 218a	0.0542	0.0686	0.3716	-0.2603
9: 206a	-> 218a	0.0352	-0.0615	0.0028	0.0264
9: 215a	-> 218a	0.0071	-0.2007	0.0138	0.0063
9: 211a	-> 218a	0.0041	0.0199	0.0124	-0.0313
9: 212a	-> 218a	0.0034	-0.0186	0.0215	0.0075
9: 217a	-> 218a	0.0008	-0.0249	0.0172	-0.0303
9: 216a	-> 218a	0.0006	-0.0172	0.0139	-0.0208
9: 205a	-> 218a	0.0006	-0.0002	-0.0003	0.0047
9: 204a	-> 218a	0.0005	0.0017	0.0092	0.0013
9: 216a	-> 220a	0.0004	-0.0023	0.0009	-0.0011
9: 215a	-> 222a	0.0003	0.0430	-0.0154	0.0069
9: 214a	-> 219a	0.0002	0.0037	-0.0069	0.0024
9: 197a	-> 218a	0.0002	0.0075	-0.0033	0.0019
9: 209a	-> 219a	0.0002	0.0054	0.0018	0.0002
9: 213a	-> 222a	0.0002	0.0219	-0.0001	-0.0137

10: 206a	-> 218a	0.6336	0.2558	-0.0116	-0.1098
10: 207a	-> 218a	0.1604	-0.1363	-0.0927	0.1662
10: 217a	-> 219a	0.0662	-0.0165	-0.0003	0.0249
10: 209a	-> 218a	0.0623	-0.3362	-0.1439	0.1467

10: 210a	-> 218a	0.0170	0.0757	0.1464	-0.0390
10: 214a	-> 218a	0.0166	0.0372	0.2018	-0.1413
10: 205a	-> 218a	0.0150	0.0011	0.0015	-0.0232
10: 213a	-> 218a	0.0133	-0.0977	0.1288	-0.0180
10: 208a	-> 218a	0.0080	-0.0248	0.0501	0.0175
10: 211a	-> 218a	0.0031	0.0170	0.0106	-0.0266
10: 204a	-> 218a	0.0013	0.0027	0.0148	0.0021
10: 203a	-> 218a	0.0005	-0.0205	-0.0421	-0.0233
10: 215a	-> 218a	0.0002	0.0296	-0.0020	-0.0009
10: 209a	-> 219a	0.0001	0.0042	0.0014	0.0002
10: 197a	-> 218a	0.0001	0.0055	-0.0024	0.0014
10: 215a	-> 221a	0.0001	-0.0067	0.0036	0.0022
10: 192a	-> 218a	0.0001	0.0007	-0.0083	-0.0018
10: 216a	-> 220a	0.0001	-0.0009	0.0004	-0.0004

Table S18 All SINGLET-TRIPLET excitation energies

no.	E/a.u.	E/eV	f	Symmetry
1:	0.02859	0.77798	0.000	A
2:	0.03203	0.87172	0.000	A
3:	0.04220	1.14827	0.000	A
4:	0.04969	1.35203	0.000	A
5:	0.05243	1.42669	0.000	A
6:	0.05447	1.48226	0.000	A
7:	0.05567	1.51494	0.000	A
8:	0.05610	1.52656	0.000	A
9:	0.05723	1.55720	0.000	A
10:	0.05845	1.59046	0.000	A

III. Computational details for [Pd(dppf)(P[*p*-C_6H_4OMe]$_3$)][BF_4]$_2$

Table S19 Optimized coordinates

1.Fe	2.550038	7.560294	3.566276
2.Pd	3.519146	10.413923	3.514040
3.P	1.404351	10.510975	2.442476
4.P	4.265974	12.601609	3.425258
5.P	5.360218	9.284103	4.381801
6.C	1.017512	8.950040	3.257320
7.C	-0.015279	11.611876	2.725193
8.C	-0.987240	11.320334	3.694719
9.H	-0.931499	10.402836	4.279147
10.C	-2.056764	12.194710	3.891144
11.H	-2.820724	11.951397	4.628689
12.C	-2.160319	13.360714	3.129676
13.H	-3.002360	14.035474	3.277683
14.C	-1.192230	13.653727	2.163557
15.H	-1.278428	14.556052	1.560555
16.C	-0.121355	12.786229	1.960525
17.H	0.617185	13.008678	1.190957
18.C	4.621548	12.952020	1.694058
19.C	3.780271	13.751238	0.905313
20.H	2.913039	14.233569	1.352864
21.C	4.043354	13.955931	-0.446748
22.H	3.383818	14.596154	-1.027369
23.C	5.160058	13.340404	-1.041619
24.H	3.685944	13.955702	-3.246186
25.C	5.996484	12.512334	-0.261252
26.H	6.858689	12.045362	-0.735504
27.C	5.728343	12.319364	1.081061
28.H	6.389215	11.680459	1.666144
29.C	5.756925	12.988965	4.382816
30.C	5.710473	12.782525	5.771067
31.H	4.837777	12.314893	6.225252
32.C	6.750396	13.189814	6.598320
33.H	6.677479	13.027961	7.670525
34.C	7.872234	13.829454	6.033605
35.H	8.849998	13.107824	8.476091
36.C	7.927481	14.038110	4.643230
37.H	8.794350	14.547659	4.225854
38.C	6.885106	13.627532	3.829499
39.H	6.940401	13.827318	2.762377
40.C	2.020242	13.272641	4.936314
41.H	1.930115	12.203177	5.126978

42.C	1.149313	14.150903	5.575368
43.H	0.390192	13.761623	6.248516
44.C	1.258218	15.530361	5.328268
45.H	-1.264593	15.371584	6.322866
46.C	2.258406	16.007007	4.455041
47.H	2.339267	17.080050	4.290549
48.C	3.132023	15.125644	3.846312
49.H	3.921018	15.518902	3.207949
50.C	7.046665	9.424036	3.717734
51.C	7.967039	10.263684	4.367373
52.H	7.688552	10.786181	5.281131
53.C	9.253842	10.414129	3.851491
54.H	9.965405	11.055396	4.368869
55.C	9.627234	9.746605	2.683359
56.H	10.634501	9.864062	2.286403
57.C	8.712609	8.915475	2.031953
58.H	9.005887	8.376698	1.132801
59.C	7.425829	8.751607	2.542822
60.H	6.737779	8.076938	2.038913
61.C	4.642063	7.769170	3.722205
62.C	4.226282	7.597121	2.338360
63.H	4.406738	8.287777	1.523317
64.C	3.576442	6.339804	2.231001
65.H	3.154664	5.919071	1.323912
66.C	3.546388	5.746191	3.533495
67.H	3.103646	4.788098	3.782992
68.C	4.189069	6.625361	4.455079
69.H	4.323005	6.459704	5.518912
70.C	5.477440	9.039498	6.177052
71.C	4.449068	9.519821	7.002351
72.H	3.623730	10.079742	6.561989
73.C	4.487523	9.290155	8.376528
74.H	3.689756	9.666470	9.014657
75.C	5.558653	8.585365	8.934741
76.H	5.592956	8.409568	10.008911
77.C	6.586909	8.109306	8.116816
78.H	7.421213	7.560545	8.550631
79.C	6.553074	8.333702	6.740800
80.H	7.358456	7.962616	6.109103
81.C	1.424160	10.160920	0.660221
82.C	2.646952	10.095914	-0.023865
83.H	3.574746	10.324066	0.501355
84.C	2.671445	9.771420	-1.380723
85.H	3.622098	9.730477	-1.911048

86.C	1.476751	9.516951	-2.059294
87.H	1.495322	9.266443	-3.118915
88.C	0.254344	9.596914	-1.383647
89.H	-0.677681	9.410603	-1.914777
90.C	0.221508	9.923580	-0.029004
91.H	-0.734117	9.998808	0.489291
92.C	1.233623	8.732033	4.680896
93.H	1.482537	9.495383	5.409924
94.C	1.003049	7.358696	4.956394
95.H	1.086794	6.879803	5.926328
96.C	0.666213	6.714833	3.723289
97.H	0.446218	5.659593	3.599929
98.C	0.678096	7.687282	2.677292
99.H	0.479750	7.505227	1.626208
100.C	3.009175	13.733983	4.058898
101.O	8.934306	14.280876	6.738664
102.H	9.818889	14.610371	8.529419
103.C	8.891182	14.161253	8.170617
104.H	8.033591	14.708129	8.582018
105.O	0.459810	16.475591	5.874932
106.H	-0.091978	15.555587	7.676025
107.C	-0.546657	16.047151	6.805550
108.H	-1.056358	16.957499	7.125277
109.O	5.514623	13.473552	-2.338178
110.H	4.713777	15.359538	-2.783889
111.C	4.713540	14.332833	-3.170634
112.H	5.187778	14.311008	-4.153231

Table S20 Selected individual LMO bond orders greater than 0.002 in magnitude, with the overlap between the hybrids in the NLMO given:

Atom I	Atom J	NLMO	Bond Order	Hybrid Overlap
1	2	101	0.0088085	0.0430187
1	2	103	0.0605933	0.1346290
1	2	108	-0.0040967	-0.0105597
1	2	109	-0.0037158	-0.0811346
1	2	118	0.0020311	0.1041524
1	2	129	0.0106575	0.1740248
1	2	145	-0.0022941	-0.0974991
1	2	201	0.0113939	0.1688076
1	2	239	0.0021227	0.0910598
1	2	259	-0.0422499	-0.0514611

Table S21 Natural localized molecular orbital (NLMO) analysis for NLMOs with a bond order greater than 0.02:

Hybridization/Polarization Analysis of NLMOs in NAO Basis:

NLMO/Occupancy/Percent from Parent NBO/ Atomic Hybrid Contributions

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103. (2.00000) 83.5718% LP (3)Fe 1

83.701% Fe 1 s(0.43%)p 0.03(0.01%)d99.99(99.56%)
3.030% Pd 2 s(16.13%)p 0.07(1.06%)d 5.13(82.81%)
0.563% P 3 s(10.57%)p 7.99(84.44%)d 0.47(4.99%)
2.498% P 4 s(33.31%)p 2.00(66.68%)d 0.00(0.01%)
1.218% P 5 s(11.52%)p 7.42(85.51%)d 0.26(2.97%)
0.527% C 6 s(0.86%)p99.99(96.58%)d 3.00(2.57%)
0.115% C 7 s(36.28%)p 1.74(63.15%)d 0.02(0.58%)
0.042% C 13 s(10.71%)p 8.30(88.92%)d 0.03(0.37%)
0.024% C 14 s(4.62%)p20.60(95.19%)d 0.04(0.19%)
0.012% C 16 s(0.36%)p99.99(99.59%)d 0.13(0.05%)
0.019% C 18 s(1.91%)p51.15(97.76%)d 0.17(0.33%)
0.036% C 19 s(23.30%)p 3.27(76.09%)d 0.03(0.61%)
0.018% C 20 s(11.00%)p 8.07(88.72%)d 0.03(0.28%)
0.019% C 24 s(12.69%)p 6.84(86.72%)d 0.05(0.59%)
0.015% C 29 s(38.71%)p 1.55(60.11%)d 0.03(1.18%)
0.089% C 30 s(32.01%)p 2.10(67.18%)d 0.03(0.81%)
0.010% C 35 s(55.23%)p 0.80(44.30%)d 0.01(0.48%)
0.978% C 36 s(0.34%)p99.99(98.12%)d 4.50(1.54%)
0.048% C 37 s(9.09%)p 7.89(71.75%)d 2.11(19.16%)
0.108% C 38 s(0.32%)p99.99(93.65%)d18.66(6.03%)
1.226% C 39 s(6.07%)p15.43(93.62%)d 0.05(0.32%)
2.016% C 40 s(0.90%)p99.99(98.99%)d 0.12(0.10%)
0.018% C 41 s(21.27%)p 3.58(76.15%)d 0.12(2.58%)
0.013% C 47 s(36.39%)p 1.69(61.45%)d 0.06(2.16%)
0.033% C 53 s(8.57%)p 7.03(60.26%)d 3.64(31.18%)
0.465% C 54 s(0.74%)p99.99(97.90%)d 1.83(1.36%)
2.019% C 55 s(5.01%)p18.95(94.89%)d 0.02(0.10%)
0.961% C 56 s(0.93%)p99.99(98.72%)d 0.38(0.35%)
0.028% C 57 s(28.16%)p 2.50(70.43%)d 0.05(1.40%)
0.014% H100 s(92.06%)p 0.09(7.94%)

Table S22 List of selected MOs, ordered by energy, with the most significant SFO gross populations

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-12.039	2.00	233 A	13.24%	2 D:yz	-4.129	2.00	2 Pd
			5.66%	1 D:xy	-7.605	1.20	1 Fe
			5.57%	2 D:xz	-4.129	2.00	2 Pd
			5.25%	1 P:x	-5.339	0.67	53 C
			4.70%	1 P:x	-5.339	0.67	37 C
			4.26%	1 P:x	-9.110	1.33	110 O
			2.94%	1 P:x	-5.339	0.67	56 C
			2.93%	1 P:x	-5.339	0.67	55 C
			2.91%	1 P:x	-5.339	0.67	39 C
			2.45%	1 D:x2-y2	-7.605	1.20	1 Fe
			2.30%	2 D:x2-y2	-4.129	2.00	2 Pd
			1.97%	1 P:x	-5.339	0.67	40 C
			1.79%	2 P:x	-5.563	1.00	3 P
			1.52%	1 P:y	-5.339	0.67	40 C
			1.45%	1 P:z	-9.110	1.33	110 O
			1.36%	3 P:z	-0.725	0.00	1 Fe
			1.13%	2 P:y	-5.563	1.00	5 P
			1.05%	1 S	-6.551	1.00	105 H
-11.988	2.00	234 A	13.13%	1 P:x	-9.110	1.33	110 O
			10.03%	1 P:y	-9.110	1.33	110 O
			6.46%	1 P:z	-9.110	1.33	110 O
			4.06%	1 S	-6.551	1.00	73 H
			3.46%	1 S	-6.551	1.00	71 H
			3.44%	1 S	-6.551	1.00	104 H
			3.39%	2 S	-24.018	2.00	110 O
			3.32%	1 P:x	-5.339	0.67	22 C
			3.02%	1 P:x	-5.339	0.67	21 C
			2.66%	1 P:x	-5.339	0.67	58 C
			2.25%	1 S	-6.551	1.00	74 H
			2.16%	1 P:y	-5.339	0.67	58 C
			1.90%	2 P:x	4.592	0.00	22 C
			1.75%	1 P:z	-5.339	0.67	58 C
			1.60%	1 P:z	-5.339	0.67	23 C
			1.40%	1 P:x	-5.339	0.67	19 C
			1.32%	2 D:xz	-4.129	2.00	2 Pd
			1.21%	1 S	-6.551	1.00	72 H
			1.19%	1 P:z	-5.339	0.67	22 C
			1.16%	1 D:xy	-7.605	1.20	1 Fe
			1.12%	1 S	-6.551	1.00	75 H

			1.12%	1 S	-6.551	1.00	105 H	
			1.10%	1 P:z	-5.339	0.67	21 C	
-11.976	2.00	235 A	26.31%	1 P:y	-9.110	1.33	111 O	
			6.31%	2 D:xz	-4.129	2.00	2 Pd	
			5.85%	1 P:y	-5.339	0.67	59 C	
			4.26%	1 P:y	-5.339	0.67	26 C	
			3.64%	2 S	-24.018	2.00	111 O	
			3.59%	1 S	-6.551	1.00	107 H	
			3.41%	1 P:y	-5.339	0.67	27 C	
			2.67%	1 S	-6.551	1.00	106 H	
			2.52%	1 S	-6.551	1.00	76 H	
			2.44%	2 D:yz	-4.129	2.00	2 Pd	
			2.30%	1 S	-6.551	1.00	78 H	
			2.24%	1 P:z	-9.110	1.33	111 O	
			2.16%	2 P:y	4.592	0.00	27 C	
			1.71%	1 S	-6.551	1.00	79 H	
			1.17%	1 P:x	-9.110	1.33	110 O	
			1.16%	1 S	-6.551	1.00	77 H	
-11.957	2.00	236 A	10.30%	1 P:z	-9.110	1.33	111 O	
			7.04%	1 P:x	-9.110	1.33	111 O	
			6.02%	1 P:z	-5.339	0.67	57 C	
			5.54%	1 P:z	-5.339	0.67	25 C	
			5.08%	1 P:x	-5.339	0.67	57 C	
			4.36%	2 D:xz	-4.129	2.00	2 Pd	
			3.96%	1 S	-6.551	1.00	106 H	
			3.50%	1 P:x	-5.339	0.67	25 C	
			3.32%	1 S	-6.551	1.00	78 H	
			2.75%	1 P:z	-5.339	0.67	29 C	
			2.57%	1 P:x	-5.339	0.67	19 C	
			2.33%	1 P:z	-5.339	0.67	59 C	
			2.32%	1 P:z	-5.339	0.67	27 C	
			2.03%	1 P:x	-5.339	0.67	27 C	
			2.01%	1 P:y	-9.110	1.33	110 O	
			1.55%	1 P:x	-5.339	0.67	59 C	
			1.46%	1 P:x	-5.339	0.67	55 C	
			1.33%	1 P:y	-5.339	0.67	24 C	
			1.32%	1 P:x	-5.339	0.67	29 C	
			1.24%	1 P:y	-9.110	1.33	112 O	
			1.19%	1 P:x	-5.339	0.67	53 C	
			1.08%	2 D:z2	-4.129	2.00	2 Pd	
			1.05%	2 D:xy	-4.129	2.00	2 Pd	
-11.861	2.00	237 A	15.97%	2 D:yz	-4.129	2.00	2 Pd	
			10.12%	2 D:xz	-4.129	2.00	2 Pd	
			9.03%	2 D:x2-y2	-4.129	2.00	2 Pd	

			6.08%	1 P:y	-9.110	1.33	111 O	
			4.87%	2 D:z2	-4.129	2.00	2 Pd	
			4.31%	1 P:x	-5.339	0.67	39 C	
			3.01%	1 P:x	-5.339	0.67	37 C	
			2.62%	1 D:x2-y2	-7.605	1.20	1 Fe	
			1.53%	1 P:x	-5.339	0.67	36 C	
			1.28%	1 P:y	-5.339	0.67	26 C	
			1.19%	1 S	-6.551	1.00	76 H	
			1.13%	1 P:y	-5.339	0.67	59 C	
			1.07%	1 P:x	-5.339	0.67	6 C	
-11.767	2.00	238 A	10.01%	2 D:x2-y2	-4.129	2.00	2 Pd	
			8.70%	2 D:xy	-4.129	2.00	2 Pd	
			8.16%	2 D:z2	-4.129	2.00	2 Pd	
			6.49%	1 P:x	-5.339	0.67	6 C	
			5.72%	1 P:x	-5.339	0.67	55 C	
			4.49%	1 P:y	-9.110	1.33	110 O	
			2.88%	1 P:y	-5.339	0.67	19 C	
			2.68%	1 P:x	-5.339	0.67	54 C	
			2.28%	2 D:yz	-4.129	2.00	2 Pd	
			2.27%	1 D:xy	-7.605	1.20	1 Fe	
			1.78%	1 P:x	-5.339	0.67	39 C	
			1.67%	1 P:x	-5.339	0.67	53 C	
			1.56%	3 P:y	-0.725	0.00	1 Fe	
			1.40%	1 P:y	-5.339	0.67	20 C	
			1.40%	1 P:x	-5.339	0.67	37 C	
			1.29%	1 P:y	-5.339	0.67	24 C	
			1.25%	1 P:x	-5.339	0.67	24 C	
			1.13%	1 S	-6.551	1.00	73 H	
			1.08%	2 P:x	-5.563	1.00	5 P	
-11.725	2.00	239 A	23.28%	2 D:z2	-4.129	2.00	2 Pd	
			20.04%	2 D:xy	-4.129	2.00	2 Pd	
			6.16%	2 D:xz	-4.129	2.00	2 Pd	
			4.20%	1 P:x	-5.339	0.67	38 C	
			3.88%	1 P:x	-5.339	0.67	36 C	
			2.58%	1 P:y	-5.339	0.67	36 C	
			2.09%	1 P:x	-5.339	0.67	39 C	
			1.92%	1 P:x	-5.339	0.67	40 C	
			1.74%	1 P:x	-5.339	0.67	56 C	
			1.57%	1 P:x	-5.339	0.67	53 C	
			1.55%	1 D:x2-y2	-7.605	1.20	1 Fe	
			1.25%	1 P:y	-5.339	0.67	38 C	
			1.18%	1 P:z	-5.339	0.67	41 C	
-11.549	2.00	240 A	9.60%	2 D:yz	-4.129	2.00	2 Pd	
			4.37%	2 D:x2-y2	-4.129	2.00	2 Pd	

				4.29%	2 D:xz	-4.129	2.00	2 Pd	
				4.12%	2 P:y	-5.563	1.00	5 P	
				3.88%	2 P:x	-5.563	1.00	3 P	
				3.14%	1 D:xy	-7.605	1.20	1 Fe	
				3.05%	1 D:x2-y2	-7.605	1.20	1 Fe	
				3.04%	1 P:x	-5.339	0.67	6 C	
				2.78%	1 P:x	-5.339	0.67	54 C	
				2.40%	1 P:x	-5.339	0.67	40 C	
				2.31%	2 D:z2	-4.129	2.00	2 Pd	
				2.19%	1 P:x	-5.339	0.67	36 C	
				1.93%	1 P:y	-5.339	0.67	44 C	
				1.92%	1 P:y	-5.339	0.67	7 C	
				1.82%	1 P:x	-5.339	0.67	38 C	
				1.55%	2 D:xy	-4.129	2.00	2 Pd	
				1.54%	1 P:x	-5.339	0.67	56 C	
				1.44%	2 P:x	-5.563	1.00	5 P	
				1.32%	1 P:y	-5.339	0.67	45 C	
				1.25%	1 P:y	-5.339	0.67	41 C	
				1.21%	1 P:y	-5.339	0.67	38 C	
				1.14%	1 P:z	-5.339	0.67	30 C	
				1.05%	1 P:z	-5.339	0.67	7 C	
				1.03%	1 P:y	-9.110	1.33	110 O	
-11.464	2.00	241	A	27.37%	2 D:yz	-4.129	2.00	2 Pd	
				8.07%	2 D:xy	-4.129	2.00	2 Pd	
				7.29%	1 P:x	-5.339	0.67	56 C	
				6.09%	1 P:x	-5.339	0.67	54 C	
				4.66%	1 P:x	-5.339	0.67	40 C	
				4.37%	1 P:x	-5.339	0.67	38 C	
				3.50%	1 P:x	-5.339	0.67	53 C	
				3.24%	2 D:x2-y2	-4.129	2.00	2 Pd	
				3.24%	1 P:x	-5.339	0.67	37 C	
				3.03%	3 P:z	-0.725	0.00	1 Fe	
				2.59%	1 P:y	-5.339	0.67	40 C	
				1.81%	2 D:xz	-4.129	2.00	2 Pd	
				1.45%	1 D:yz	-7.605	1.20	1 Fe	
				1.44%	1 P:y	-5.339	0.67	37 C	
				1.38%	1 P:x	-5.339	0.67	39 C	
-11.189	2.00	242	A	16.86%	1 P:y	-5.339	0.67	44 C	
				15.96%	1 P:y	-5.339	0.67	41 C	
				7.68%	1 P:y	-5.339	0.67	43 C	
				5.92%	1 P:x	-5.339	0.67	44 C	
				5.30%	1 P:x	-5.339	0.67	41 C	
				3.79%	1 P:y	-5.339	0.67	46 C	
				3.51%	1 P:y	-5.339	0.67	45 C	

			3.04%	1 P:y	-5.339	0.67	33 C	
			2.61%	1 P:x	-5.339	0.67	43 C	
			2.50%	1 P:y	-5.339	0.67	30 C	
			2.25%	1 P:y	-5.339	0.67	34 C	
			1.91%	1 P:z	-5.339	0.67	33 C	
			1.36%	2 D:z2	-4.129	2.00	2 Pd	
			1.22%	1 P:y	-5.339	0.67	31 C	
			1.21%	1 P:y	-5.339	0.67	36 C	
			1.18%	1 P:x	-5.339	0.67	45 C	
			1.16%	1 P:z	-5.339	0.67	34 C	
			1.12%	1 P:z	-5.339	0.67	30 C	
			1.04%	2 D:xy	-4.129	2.00	2 Pd	
			1.00%	1 P:x	-5.339	0.67	46 C	
-11.135	2.00	243 A	16.66%	2 D:z2	-4.129	2.00	2 Pd	
			12.42%	2 D:xz	-4.129	2.00	2 Pd	
			3.84%	1 P:z	-5.339	0.67	10 C	
			3.51%	1 P:z	-5.339	0.67	7 C	
			2.43%	1 P:y	-5.339	0.67	7 C	
			2.23%	1 P:y	-5.339	0.67	50 C	
			2.07%	2 P:x	-5.563	1.00	3 P	
			1.97%	1 P:x	-5.339	0.67	10 C	
			1.97%	1 P:y	-5.339	0.67	15 C	
			1.93%	1 P:y	-5.339	0.67	10 C	
			1.79%	1 P:y	-5.339	0.67	44 C	
			1.73%	1 P:y	-5.339	0.67	47 C	
			1.68%	1 P:y	-5.339	0.67	41 C	
			1.67%	1 P:y	-5.339	0.67	30 C	
			1.63%	1 P:y	-5.339	0.67	14 C	
			1.59%	1 P:z	-5.339	0.67	9 C	
			1.54%	1 P:y	-5.339	0.67	33 C	
			1.29%	5 S	-3.388	0.00	2 Pd	
			1.19%	1 P:z	-5.339	0.67	30 C	
			1.15%	1 P:x	-5.339	0.67	9 C	
			1.12%	1 P:y	-5.339	0.67	32 C	
			1.08%	1 P:x	-5.339	0.67	7 C	
			1.07%	1 P:y	-5.339	0.67	49 C	
			1.01%	1 P:z	-5.339	0.67	11 C	
			1.00%	2 D:yz	-4.129	2.00	2 Pd	
-11.062	2.00	244 A	17.86%	1 P:y	-5.339	0.67	42 C	
			16.88%	1 P:y	-5.339	0.67	45 C	
			16.08%	1 P:y	-5.339	0.67	46 C	
			12.34%	1 P:y	-5.339	0.67	43 C	
			6.14%	1 P:x	-5.339	0.67	42 C	
			5.82%	1 P:x	-5.339	0.67	45 C	

			5.00%	1 P:x	-5.339	0.67	46 C	
			4.24%	1 P:x	-5.339	0.67	43 C	
-11.005	2.00	245 A	20.96%	1 P:y	-5.339	0.67	50 C	
			19.58%	1 P:y	-5.339	0.67	47 C	
			11.13%	1 P:y	-5.339	0.67	49 C	
			6.15%	1 P:y	-5.339	0.67	52 C	
			4.69%	2 D:z2	-4.129	2.00	2 Pd	
			3.26%	1 P:y	-5.339	0.67	51 C	
			3.21%	2 D:xz	-4.129	2.00	2 Pd	
			1.54%	1 P:z	-5.339	0.67	47 C	
			1.48%	1 P:x	-5.339	0.67	7 C	
			1.23%	1 P:z	-5.339	0.67	9 C	
			1.12%	1 P:z	-5.339	0.67	50 C	
-10.978	2.00	246 A	10.23%	1 P:y	-5.339	0.67	18 C	
			9.41%	1 P:y	-5.339	0.67	15 C	
			8.61%	1 P:y	-5.339	0.67	14 C	
			7.79%	1 P:y	-5.339	0.67	17 C	
			5.45%	1 P:x	-5.339	0.67	18 C	
			4.60%	1 P:x	-5.339	0.67	15 C	
			4.38%	1 P:x	-5.339	0.67	14 C	
			3.83%	1 P:x	-5.339	0.67	17 C	
			3.73%	1 P:y	-5.339	0.67	51 C	
			3.57%	1 P:y	-5.339	0.67	48 C	
			2.09%	1 P:y	-5.339	0.67	30 C	
			2.04%	1 P:y	-5.339	0.67	33 C	
			1.34%	1 P:y	-5.339	0.67	50 C	
			1.17%	1 P:z	-5.339	0.67	30 C	
			1.16%	1 P:y	-5.339	0.67	47 C	
			1.11%	1 P:y	-5.339	0.67	34 C	
			1.04%	1 P:y	-5.339	0.67	52 C	
			1.03%	1 P:z	-5.339	0.67	33 C	
-10.868	2.00	247 A	6.95%	1 P:y	-5.339	0.67	48 C	
			6.89%	1 P:y	-5.339	0.67	51 C	
			5.78%	1 P:y	-5.339	0.67	21 C	
			5.03%	1 P:y	-5.339	0.67	20 C	
			4.33%	1 P:y	-5.339	0.67	32 C	
			4.00%	1 P:y	-5.339	0.67	52 C	
			3.85%	2 D:z2	-4.129	2.00	2 Pd	
			3.77%	1 P:y	-5.339	0.67	35 C	
			2.83%	1 P:y	-5.339	0.67	24 C	
			2.78%	2 D:xz	-4.129	2.00	2 Pd	
			2.76%	1 P:y	-5.339	0.67	49 C	
			2.39%	1 P:z	-5.339	0.67	35 C	
			2.38%	1 P:z	-5.339	0.67	32 C	

			2.37%	2	P:y	-5.563	1.00	4	P
			2.35%	1	P:y	-5.339	0.67	17	C
			2.00%	1	P:y	-5.339	0.67	18	C
			1.65%	1	P:x	-5.339	0.67	21	C
			1.59%	1	P:y	-5.339	0.67	23	C
			1.47%	1	P:y	-5.339	0.67	33	C
			1.45%	1	P:y	-5.339	0.67	31	C
			1.26%	2	D:x2-y2	-4.129	2.00	2	Pd
			1.22%	1	P:y	-5.339	0.67	30	C
			1.22%	1	P:x	-5.339	0.67	17	C
			1.15%	5	S	-3.388	0.00	2	Pd
			1.09%	1	P:y	-5.339	0.67	14	C
			1.06%	1	P:x	-5.339	0.67	20	C
			1.02%	1	P:x	-5.339	0.67	18	C
-10.836	2.00	248	A	13.00%	1	P:y	-5.339	0.67	48 C
			12.37%	1	P:y	-5.339	0.67	51	C
			11.15%	1	P:y	-5.339	0.67	52	C
			9.17%	1	P:y	-5.339	0.67	49	C
			2.09%	1	P:z	-5.339	0.67	11	C
			2.04%	2	D:z2	-4.129	2.00	2	Pd
			1.91%	1	P:y	-5.339	0.67	21	C
			1.82%	1	P:z	-5.339	0.67	8	C
			1.65%	1	P:y	-5.339	0.67	20	C
			1.59%	1	P:y	-5.339	0.67	32	C
			1.30%	1	P:y	-5.339	0.67	35	C
			1.21%	1	P:y	-5.339	0.67	11	C
			1.21%	1	P:x	-5.339	0.67	11	C
			1.16%	1	P:x	-5.339	0.67	8	C
			1.10%	1	P:y	-5.339	0.67	8	C
			1.06%	1	P:y	-5.339	0.67	15	C
-10.808	2.00	249	A	8.22%	1	P:y	-5.339	0.67	31 C
			8.10%	1	P:y	-5.339	0.67	34	C
			4.10%	1	P:z	-5.339	0.67	34	C
			3.94%	1	P:z	-5.339	0.67	31	C
			3.73%	1	P:y	-5.339	0.67	35	C
			3.55%	1	P:y	-5.339	0.67	17	C
			2.98%	1	P:y	-5.339	0.67	32	C
			2.85%	1	P:y	-5.339	0.67	18	C
			2.76%	2	D:z2	-4.129	2.00	2	Pd
			2.28%	1	P:y	-5.339	0.67	23	C
			2.13%	1	P:z	-5.339	0.67	35	C
			1.96%	1	P:y	-5.339	0.67	24	C
			1.86%	2	P:y	-5.563	1.00	4	P
			1.72%	1	P:x	-5.339	0.67	17	C

			1.67%	1 P:y	-5.339	0.67	14 C		
			1.63%	1 P:x	-5.339	0.67	18 C		
			1.61%	1 P:y	-5.339	0.67	20 C		
			1.54%	2 D:xz	-4.129	2.00	2 Pd		
			1.44%	1 P:z	-5.339	0.67	32 C		
			1.41%	1 P:y	-5.339	0.67	21 C		
			1.38%	1 P:x	-5.339	0.67	34 C		
			1.21%	1 P:x	-5.339	0.67	31 C		
			1.11%	1 P:z	-5.339	0.67	11 C		
			1.08%	1 P:y	-5.339	0.67	30 C		
			1.06%	2 D:x2-y2	-4.129	2.00	2 Pd		
			1.06%	1 P:y	-5.339	0.67	33 C		
			1.02%	5 S	-3.388	0.00	2 Pd		
			1.01%	1 P:z	-5.339	0.67	10 C		
-10.705	2.00	250 A	10.06%	1 P:z	-5.339	0.67	8 C		
			8.72%	1 P:z	-5.339	0.67	12 C		
			8.67%	1 P:z	-5.339	0.67	11 C		
			7.82%	1 P:z	-5.339	0.67	9 C		
			5.54%	1 P:x	-5.339	0.67	12 C		
			5.43%	1 P:x	-5.339	0.67	11 C		
			5.34%	1 P:x	-5.339	0.67	8 C		
			4.83%	1 P:y	-5.339	0.67	12 C		
			4.75%	1 P:x	-5.339	0.67	9 C		
			4.67%	1 P:y	-5.339	0.67	11 C		
			4.63%	1 P:y	-5.339	0.67	8 C		
			3.85%	1 P:y	-5.339	0.67	9 C		
			3.76%	1 P:y	-5.339	0.67	49 C		
			3.58%	1 P:y	-5.339	0.67	52 C		
			1.80%	1 P:y	-5.339	0.67	48 C		
			1.75%	1 P:y	-5.339	0.67	51 C		
-10.655	2.00	251 A	9.01%	1 P:y	-5.339	0.67	24 C		
			7.11%	1 P:y	-5.339	0.67	21 C		
			7.09%	1 P:y	-5.339	0.67	23 C		
			6.45%	1 P:y	-5.339	0.67	20 C		
			5.60%	1 P:y	-5.339	0.67	32 C		
			5.48%	1 P:y	-5.339	0.67	35 C		
			3.78%	1 P:z	-5.339	0.67	29 C		
			2.72%	1 P:x	-5.339	0.67	24 C		
			2.69%	1 P:z	-5.339	0.67	26 C		
			2.67%	1 P:z	-5.339	0.67	35 C		
			2.67%	1 P:z	-5.339	0.67	28 C		
			2.42%	1 P:z	-5.339	0.67	32 C		
			2.35%	1 P:z	-5.339	0.67	25 C		
			2.29%	1 P:x	-5.339	0.67	29 C		

			2.01%	1 P:x	-5.339	0.67	21 C		
			1.91%	1 P:y	-5.339	0.67	31 C		
			1.80%	1 P:x	-5.339	0.67	28 C		
			1.76%	1 P:x	-5.339	0.67	26 C		
			1.75%	1 P:x	-5.339	0.67	25 C		
			1.66%	1 P:x	-5.339	0.67	23 C		
			1.49%	1 P:y	-5.339	0.67	34 C		
			1.39%	1 P:z	-5.339	0.67	31 C		
			1.32%	1 P:x	-5.339	0.67	20 C		
			1.22%	5 S	-3.388	0.00	2 Pd		
			1.15%	1 P:y	-5.339	0.67	33 C		
-10.610	2.00	252 A	11.36%	1 P:z	-5.339	0.67	29 C		
			9.69%	1 P:z	-5.339	0.67	26 C		
			8.25%	1 P:z	-5.339	0.67	28 C		
			8.10%	1 P:z	-5.339	0.67	25 C		
			6.50%	1 P:x	-5.339	0.67	26 C		
			6.38%	1 P:x	-5.339	0.67	29 C		
			6.07%	1 P:x	-5.339	0.67	25 C		
			5.45%	1 P:x	-5.339	0.67	28 C		
			4.44%	1 P:y	-5.339	0.67	24 C		
			3.26%	1 P:y	-5.339	0.67	23 C		
			3.00%	1 P:y	-5.339	0.67	21 C		
			2.34%	1 P:y	-5.339	0.67	20 C		
			1.56%	1 P:y	-5.339	0.67	31 C		
			1.54%	1 P:y	-5.339	0.67	34 C		
			1.10%	1 P:z	-5.339	0.67	31 C		
			1.02%	1 P:x	-5.339	0.67	23 C		
-10.436	2.00	253 A	5.16%	1 P:z	-5.339	0.67	10 C		
			4.69%	1 P:z	-5.339	0.67	7 C		
			4.27%	1 P:y	-5.339	0.67	33 C		
			3.98%	1 P:x	-5.339	0.67	7 C		
			3.79%	1 P:y	-5.339	0.67	30 C		
			3.16%	1 P:x	-5.339	0.67	10 C		
			2.75%	1 P:y	-5.339	0.67	10 C		
			2.69%	1 P:y	-5.339	0.67	47 C		
			2.43%	2 P:x	-5.563	1.00	3 P		
			2.32%	1 P:z	-5.339	0.67	12 C		
			2.23%	1 P:z	-5.339	0.67	9 C		
			2.18%	2 P:y	-5.563	1.00	5 P		
			1.97%	1 P:y	-5.339	0.67	7 C		
			1.95%	1 P:y	-5.339	0.67	50 C		
			1.89%	1 P:z	-5.339	0.67	33 C		
			1.80%	4 P:x	0.627	0.00	2 Pd		
			1.73%	1 P:y	-5.339	0.67	31 C		

			1.73%	1 D:yz	-7.605	1.20	1 Fe	
			1.71%	2 P:x	-5.563	1.00	5 P	
			1.70%	3 S	-14.037	2.00	5 P	
			1.66%	1 P:y	-5.339	0.67	34 C	
			1.55%	1 P:z	-5.339	0.67	30 C	
			1.49%	3 S	-14.037	2.00	3 P	
			1.24%	1 P:y	-5.339	0.67	49 C	
			1.24%	4 P:z	0.627	0.00	2 Pd	
			1.23%	1 P:y	-5.339	0.67	9 C	
			1.19%	1 P:z	-5.339	0.67	31 C	
			1.17%	1 P:y	-5.339	0.67	52 C	
			1.16%	1 P:x	-5.339	0.67	12 C	
			1.16%	1 P:y	-5.339	0.67	12 C	
			1.15%	1 P:x	-5.339	0.67	30 C	
			1.12%	1 P:y	-5.339	0.67	41 C	
			1.07%	1 P:x	-5.339	0.67	9 C	
-10.300	2.00	254 A	33.91%	1 D:x2-y2	-7.605	1.20	1 Fe	
			21.30%	1 D:xy	-7.605	1.20	1 Fe	
			5.75%	5 S	-3.388	0.00	2 Pd	
			4.13%	2 D:xz	-4.129	2.00	2 Pd	
			1.42%	1 D:xz	-7.605	1.20	1 Fe	
			1.39%	4 P:y	0.627	0.00	2 Pd	
			1.33%	1 P:y	-5.339	0.67	6 C	
			1.21%	2 P:y	-5.563	1.00	4 P	
			1.10%	1 P:x	-5.339	0.67	36 C	
			1.02%	1 P:y	-9.110	1.33	110 O	
-9.921	2.00	255 A	8.90%	1 P:y	-9.110	1.33	110 O	
			5.99%	1 P:y	-9.110	1.33	112 O	
			5.97%	1 P:y	-5.339	0.67	19 C	
			5.15%	1 P:y	-5.339	0.67	13 C	
			4.66%	1 P:z	-9.110	1.33	111 O	
			4.01%	1 P:y	-5.339	0.67	21 C	
			3.72%	1 P:z	-5.339	0.67	57 C	
			3.46%	1 P:y	-5.339	0.67	23 C	
			3.30%	1 P:x	-9.110	1.33	111 O	
			3.23%	1 P:x	-9.110	1.33	112 O	
			3.19%	1 P:y	-5.339	0.67	17 C	
			2.86%	1 P:y	-5.339	0.67	22 C	
			2.84%	1 P:z	-5.339	0.67	28 C	
			2.47%	1 P:y	-5.339	0.67	15 C	
			2.47%	1 P:x	-5.339	0.67	13 C	
			2.42%	1 P:y	-5.339	0.67	16 C	
			2.32%	1 P:x	-5.339	0.67	28 C	
			2.15%	1 P:x	-9.110	1.33	110 O	

			1.51%	1 P:x	-5.339	0.67	17 C	
			1.31%	1 D:z2	-7.605	1.20	1 Fe	
			1.30%	1 P:z	-5.339	0.67	27 C	
			1.27%	1 P:x	-5.339	0.67	23 C	
			1.20%	1 P:x	-5.339	0.67	16 C	
			1.17%	1 P:z	-5.339	0.67	26 C	
			1.14%	1 P:x	-5.339	0.67	15 C	
			1.13%	1 P:x	-5.339	0.67	26 C	
			1.04%	1 P:x	-5.339	0.67	19 C	
			1.01%	1 P:x	-5.339	0.67	21 C	
-9.880	2.00	256 A	54.57%	1 D:z2	-7.605	1.20	1 Fe	
			6.72%	1 D:xz	-7.605	1.20	1 Fe	
			2.56%	1 P:y	-9.110	1.33	112 O	
			2.26%	4 S	-5.371	2.00	1 Fe	
			2.07%	1 P:y	-5.339	0.67	13 C	
			1.88%	1 D:x2-y2	-7.605	1.20	1 Fe	
			1.73%	1 P:x	-5.339	0.67	55 C	
			1.45%	1 P:x	-9.110	1.33	112 O	
			1.42%	1 D:yz	-7.605	1.20	1 Fe	
			1.37%	1 P:y	-5.339	0.67	15 C	
			1.27%	1 P:x	-5.339	0.67	40 C	
			1.13%	1 P:x	-5.339	0.67	39 C	
			1.10%	1 P:y	-5.339	0.67	16 C	
			1.07%	1 P:x	-5.339	0.67	13 C	
			1.07%	1 P:y	-5.339	0.67	17 C	
-9.824	2.00	257 A	19.29%	1 D:yz	-7.605	1.20	1 Fe	
			12.51%	1 D:z2	-7.605	1.20	1 Fe	
			5.74%	1 D:xz	-7.605	1.20	1 Fe	
			5.28%	1 D:x2-y2	-7.605	1.20	1 Fe	
			3.16%	1 P:y	-9.110	1.33	112 O	
			2.55%	1 P:y	-5.339	0.67	13 C	
			2.43%	1 P:z	-5.339	0.67	57 C	
			2.36%	1 P:x	-5.339	0.67	6 C	
			2.13%	1 P:y	-5.339	0.67	19 C	
			2.08%	1 P:y	-9.110	1.33	110 O	
			2.06%	1 P:z	-9.110	1.33	111 O	
			1.84%	1 P:x	-9.110	1.33	112 O	
			1.67%	1 P:y	-5.339	0.67	15 C	
			1.51%	1 P:x	-9.110	1.33	111 O	
			1.44%	1 P:y	-5.339	0.67	16 C	
			1.37%	1 P:x	-5.339	0.67	37 C	
			1.32%	1 P:y	-5.339	0.67	17 C	
			1.29%	1 P:x	-5.339	0.67	13 C	
-9.766	2.00	258 A	45.07%	1 D:yz	-7.605	1.20	1 Fe	

			5.21%	1 D:z2	-7.605	1.20	1 Fe	
			3.80%	1 D:xy	-7.605	1.20	1 Fe	
			3.25%	1 D:xz	-7.605	1.20	1 Fe	
			2.50%	1 P:x	-5.339	0.67	36 C	
			2.36%	1 P:y	-9.110	1.33	112 O	
			2.33%	1 P:x	-5.339	0.67	53 C	
			2.00%	1 P:y	-5.339	0.67	13 C	
			1.43%	1 P:x	-5.339	0.67	37 C	
			1.37%	1 P:x	-9.110	1.33	112 O	
			1.37%	2 D:yz	-4.129	2.00	2 Pd	
			1.29%	1 P:z	-5.339	0.67	57 C	
			1.29%	1 P:y	-5.339	0.67	15 C	
			1.20%	1 P:z	-9.110	1.33	111 O	
			1.17%	1 P:y	-5.339	0.67	16 C	
			1.12%	1 P:x	-5.339	0.67	13 C	
-9.568	2.00	259 A	9.23%	1 P:y	-9.110	1.33	110 O	
			8.05%	1 P:z	-9.110	1.33	111 O	
			7.02%	1 P:y	-5.339	0.67	19 C	
			5.97%	1 P:x	-5.339	0.67	57 C	
			5.96%	1 P:z	-5.339	0.67	57 C	
			5.95%	1 P:x	-9.110	1.33	111 O	
			5.52%	1 P:y	-5.339	0.67	23 C	
			4.44%	1 P:y	-5.339	0.67	22 C	
			4.43%	1 P:z	-5.339	0.67	26 C	
			3.83%	1 P:z	-5.339	0.67	27 C	
			3.50%	1 P:z	-5.339	0.67	28 C	
			2.87%	1 P:x	-5.339	0.67	19 C	
			2.83%	1 P:x	-5.339	0.67	26 C	
			2.66%	1 P:y	-5.339	0.67	21 C	
			2.60%	1 P:x	-5.339	0.67	27 C	
			2.19%	1 P:x	-9.110	1.33	110 O	
			2.17%	1 P:x	-5.339	0.67	28 C	
			1.48%	1 P:y	-5.339	0.67	20 C	
			1.17%	1 P:x	-5.339	0.67	23 C	
			1.11%	1 P:x	-5.339	0.67	22 C	
			1.06%	1 S	-6.551	1.00	78 H	
			1.05%	1 S	-6.551	1.00	106 H	
-8.125	0.00	260 A	12.29%	2 P:y	-5.563	1.00	4 P	
			12.01%	2 D:x2-y2	-4.129	2.00	2 Pd	
			7.12%	2 D:xy	-4.129	2.00	2 Pd	
			5.44%	2 P:y	-5.563	1.00	5 P	
			5.13%	2 P:x	-5.563	1.00	3 P	
			4.90%	3 S	-14.037	2.00	4 P	
			3.51%	1 D:x2-y2	-7.605	1.20	1 Fe	

			3.50%	3 S	-14.037	2.00	5 P	
			3.45%	1 D:xy	-7.605	1.20	1 Fe	
			3.30%	2 D:xz	-4.129	2.00	2 Pd	
			3.23%	3 S	-14.037	2.00	3 P	
			2.38%	2 P:x	-5.563	1.00	5 P	
			1.67%	1 P:x	-5.339	0.67	53 C	
			-1.44%	3 D:x2-y2	5.439	0.00	2 Pd	
			1.19%	1 D:z2	-7.605	1.20	1 Fe	
			-1.18%	4 S	3.043	0.00	4 P	
			1.15%	1 P:x	-5.339	0.67	37 C	
			1.06%	2 P:x	-5.563	1.00	4 P	
			1.05%	4 P:y	0.627	0.00	2 Pd	
-7.267	0.00	261 A	28.47%	1 D:xy	-7.605	1.20	1 Fe	
			20.41%	1 D:x2-y2	-7.605	1.20	1 Fe	
			8.27%	1 P:x	-5.339	0.67	55 C	
			6.68%	1 P:x	-5.339	0.67	36 C	
			5.73%	1 P:x	-5.339	0.67	39 C	
			3.99%	1 P:x	-5.339	0.67	6 C	
			3.98%	1 P:x	-5.339	0.67	53 C	
			2.72%	1 P:x	-5.339	0.67	38 C	
			2.04%	1 D:yz	-7.605	1.20	1 Fe	
			1.98%	1 P:y	-5.339	0.67	39 C	
			1.31%	1 P:y	-5.339	0.67	36 C	
			1.15%	1 P:x	-5.339	0.67	56 C	

Table S23 Excitation energies E in a.u. and eV, dE wrt prev. cycle, oscillator strengths f in a.u.

no.	E/a.u.	E/eV	f	dE/a.u.	
1	0.25349E-01	0.68978		0.17986E-02	0.63E-09
2	0.47926E-01	1.3041		0.93097E-01	0.55E-07
3	0.52587E-01	1.4310		0.62992E-03	0.18E-09
4	0.53499E-01	1.4558		0.55054E-01	0.16E-07
5	0.54023E-01	1.4700		0.86084E-01	0.27E-07
6	0.57768E-01	1.5719		0.13852E-01	0.14E-07
7	0.60971E-01	1.6591		0.10382E-01	0.16E-08
8	0.63249E-01	1.7211		0.16780E-02	0.25E-08
9	0.64643E-01	1.7590		0.13228E-01	0.14E-07
10	0.71751E-01	1.9524		0.56744E-02	0.46E-08

Table S24 Transition dipole moments mu (x,y,z) in a.u. (weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	0.68978	0.17986E-02	-0.29440	-0.87924E-01	-0.10968
2	1.3041	0.93097E-01	0.54236	-0.31496E-01	1.6182
3	1.4310	0.62992E-03	0.46945E-02	0.10235	-0.86428E-01
4	1.4558	0.55054E-01	0.59664	1.0017	-0.42931
5	1.4700	0.86084E-01	-0.68807	-1.3149	0.43337
6	1.5719	0.13852E-01	-0.48763	-0.23100	-0.26181
7	1.6591	0.10382E-01	0.39435	-0.44603E-01	0.31294
8	1.7211	0.16780E-02	0.33665E-01	-0.14592	0.13179
9	1.7590	0.13228E-01	-0.27115E-01	-0.44601	0.32755
10	1.9524	0.56744E-02	0.33554	-0.16982E-01	0.75855E-01

Table S25 Major MO -> MO transitions for the above excitations

Excitation Nr.	Occupied to virtual orbitals	Contribution weight (sum=1)	contribibutions to transition dipole moment x	y	z
1: 259a	-> 260a	0.9878	-0.7935	-0.3501	-0.4760
1: 257a	-> 260a	0.0101	0.2905	0.3318	0.1021
1: 258a	-> 260a	0.0016	-0.0279	-0.0959	0.1740
2: 258a	-> 260a	0.6346	-0.3996	-1.3713	2.4882
2: 257a	-> 260a	0.3332	1.2111	1.3832	0.4257
2: 259a	-> 260a	0.0080	0.0519	0.0229	0.0311
2: 258a	-> 263a	0.0046	0.0460	0.0490	-0.1170
2: 258a	-> 262a	0.0039	-0.0098	0.0302	-0.0249
2: 258a	-> 261a	0.0024	-0.0020	0.0088	-0.0146
2: 259a	-> 261a	0.0022	-0.0026	0.0004	-0.0012
2: 258a	-> 264a	0.0010	0.0115	0.0143	-0.0351
2: 258a	-> 274a	0.0010	0.0121	0.0154	-0.0852
2: 257a	-> 264a	0.0006	-0.0322	-0.0363	-0.0161
2: 257a	-> 269a	0.0006	-0.0193	-0.0126	-0.0409
2: 257a	-> 267a	0.0004	-0.0178	-0.0071	-0.0293
2: 257a	-> 270a	0.0003	-0.0130	-0.0081	-0.0158
2: 258a	-> 278a	0.0003	-0.0049	-0.0060	-0.0236
2: 258a	-> 265a	0.0003	-0.0056	-0.0002	-0.0209
2: 257a	-> 268a	0.0003	-0.0198	-0.0025	-0.0101
2: 256a	-> 260a	0.0003	-0.0171	0.0060	-0.0146
2: 259a	-> 264a	0.0002	-0.0143	0.0069	0.0019
2: 259a	-> 269a	0.0002	-0.0197	-0.0051	-0.0015
2: 257a	-> 261a	0.0002	-0.0006	-0.0020	-0.0007
3: 259a	-> 261a	0.9948	-0.0526	0.0084	-0.0246
3: 258a	-> 260a	0.0044	0.0317	0.1087	-0.1972
4: 259a	-> 262a	0.5847	-0.0156	-0.1492	-0.0276
4: 257a	-> 260a	0.2509	0.9946	1.1360	0.3496
4: 258a	-> 260a	0.1264	0.1688	0.5794	-1.0513
4: 256a	-> 260a	0.0161	-0.1289	0.0452	-0.1102

4: 258a	-> 262a	0.0064	0.0118	-0.0364	0.0301
4: 258a	-> 263a	0.0026	-0.0327	-0.0349	0.0833
4: 259a	-> 261a	0.0021	0.0024	-0.0004	0.0011
4: 258a	-> 261a	0.0021	0.0018	-0.0078	0.0129
4: 259a	-> 260a	0.0012	0.0193	0.0085	0.0116
4: 257a	-> 264a	0.0007	-0.0317	-0.0357	-0.0158
4: 251a	-> 260a	0.0005	-0.0195	0.0030	0.0165
4: 258a	-> 274a	0.0005	-0.0077	-0.0098	0.0542
4: 245a	-> 260a	0.0004	-0.0138	-0.0474	-0.0047
4: 257a	-> 261a	0.0004	-0.0008	-0.0027	-0.0009
4: 258a	-> 264a	0.0003	-0.0058	-0.0072	0.0178
4: 246a	-> 260a	0.0002	0.0059	-0.0236	-0.0024
4: 255a	-> 260a	0.0002	-0.0077	0.0045	-0.0075
4: 237a	-> 260a	0.0002	-0.0018	-0.0118	-0.0011
4: 258a	-> 269a	0.0002	-0.0157	-0.0006	0.0025
4: 239a	-> 260a	0.0001	-0.0067	-0.0056	-0.0081

5: 259a	-> 262a	0.4145	-0.0131	-0.1250	-0.0231
5: 257a	-> 260a	0.3478	-1.1655	-1.3311	-0.4097
5: 258a	-> 260a	0.1732	-0.1966	-0.6748	1.2244
5: 256a	-> 260a	0.0331	0.1840	-0.0645	0.1573
5: 258a	-> 262a	0.0096	-0.0145	0.0445	-0.0368
5: 258a	-> 263a	0.0039	0.0400	0.0427	-0.1018
5: 258a	-> 261a	0.0036	-0.0023	0.0102	-0.0170
5: 259a	-> 260a	0.0017	-0.0225	-0.0099	-0.0135
5: 257a	-> 264a	0.0011	0.0410	0.0462	0.0204
5: 245a	-> 260a	0.0009	0.0200	0.0688	0.0068
5: 259a	-> 261a	0.0008	-0.0015	0.0002	-0.0007
5: 251a	-> 260a	0.0007	0.0237	-0.0036	-0.0201
5: 258a	-> 274a	0.0007	0.0093	0.0118	-0.0655
5: 257a	-> 261a	0.0006	0.0011	0.0035	0.0012
5: 246a	-> 260a	0.0005	-0.0085	0.0340	0.0035
5: 258a	-> 264a	0.0005	0.0073	0.0091	-0.0224
5: 237a	-> 260a	0.0003	0.0021	0.0140	0.0013
5: 258a	-> 269a	0.0003	0.0185	0.0007	-0.0029
5: 255a	-> 260a	0.0002	0.0078	-0.0046	0.0075
5: 252a	-> 260a	0.0002	-0.0205	0.0082	0.0006

6: 256a	-> 260a	0.7980	-0.8738	0.3065	-0.7471
6: 255a	-> 260a	0.1592	0.1998	-0.1169	0.1935
6: 257a	-> 260a	0.0258	-0.3070	-0.3506	-0.1079
6: 258a	-> 260a	0.0085	-0.0420	-0.1442	0.2616

6: 254a	-> 260a	0.0012	0.0443	-0.0103	0.0097
6: 258a	-> 262a	0.0010	-0.0045	0.0139	-0.0115
6: 251a	-> 260a	0.0009	0.0257	-0.0039	-0.0218
6: 258a	-> 261a	0.0006	-0.0009	0.0041	-0.0067
6: 252a	-> 260a	0.0006	0.0334	-0.0134	-0.0010
6: 258a	-> 263a	0.0004	0.0120	0.0128	-0.0306
6: 259a	-> 262a	0.0004	-0.0004	-0.0036	-0.0007
6: 257a	-> 264a	0.0003	0.0195	0.0220	0.0097
6: 259a	-> 260a	0.0002	-0.0081	-0.0036	-0.0048
6: 253a	-> 260a	0.0002	0.0216	-0.0013	0.0016
6: 257a	-> 261a	0.0001	0.0005	0.0016	0.0005
6: 256a	-> 264a	0.0001	0.0118	-0.0064	0.0118
6: 255a	-> 261a	0.0001	0.0021	0.0000	0.0034
6: 258a	-> 264a	0.0001	0.0029	0.0036	-0.0088
6: 239a	-> 260a	0.0001	0.0048	0.0041	0.0059
6: 256a	-> 275a	0.0001	0.0020	-0.0041	0.0134

7: 255a	-> 260a	0.8316	0.4445	-0.2601	0.4306
7: 256a	-> 260a	0.1413	0.3579	-0.1255	0.3060
7: 254a	-> 260a	0.0088	-0.1163	0.0271	-0.0253
7: 257a	-> 260a	0.0062	0.1460	0.1668	0.0513
7: 258a	-> 260a	0.0032	0.0250	0.0859	-0.1559
7: 258a	-> 261a	0.0018	0.0015	-0.0068	0.0113
7: 251a	-> 260a	0.0013	-0.0304	0.0047	0.0257
7: 252a	-> 260a	0.0011	-0.0446	0.0178	0.0013
7: 253a	-> 260a	0.0009	-0.0432	0.0026	-0.0032
7: 255a	-> 261a	0.0003	-0.0036	0.0000	-0.0059
7: 258a	-> 262a	0.0002	0.0021	-0.0066	0.0054
7: 258a	-> 263a	0.0002	-0.0087	-0.0093	0.0222
7: 236a	-> 260a	0.0001	-0.0031	0.0053	-0.0067
7: 255a	-> 264a	0.0001	-0.0054	0.0020	-0.0108
7: 256a	-> 264a	0.0001	-0.0110	0.0059	-0.0109
7: 257a	-> 264a	0.0001	-0.0123	-0.0139	-0.0061
7: 257a	-> 262a	0.0001	-0.0037	0.0012	-0.0003
7: 255a	-> 272a	0.0001	0.0065	-0.0020	-0.0153
7: 257a	-> 261a	0.0001	-0.0004	-0.0012	-0.0004
7: 255a	-> 262a	0.0001	-0.0001	-0.0009	-0.0012

8: 258a	-> 261a	0.9556	0.0347	-0.1532	0.2546
8: 258a	-> 262a	0.0332	-0.0248	0.0765	-0.0632
8: 257a	-> 261a	0.0041	0.0026	0.0084	0.0028
8: 258a	-> 260a	0.0036	-0.0261	-0.0897	0.1628

8: 255a	-> 260a	0.0007	-0.0126	0.0074	-0.0122
8: 257a	-> 260a	0.0005	-0.0417	-0.0476	-0.0147
8: 256a	-> 260a	0.0004	-0.0185	0.0065	-0.0158
9: 258a	-> 262a	0.9410	0.1308	-0.4026	0.3325
9: 258a	-> 261a	0.0282	0.0059	-0.0260	0.0432
9: 258a	-> 260a	0.0175	-0.0571	-0.1960	0.3557
9: 257a	-> 260a	0.0051	-0.1293	-0.1477	-0.0455
9: 257a	-> 262a	0.0027	-0.0196	0.0066	-0.0016
9: 258a	-> 263a	0.0014	0.0220	0.0235	-0.0561
9: 257a	-> 261a	0.0007	0.0011	0.0035	0.0011
9: 251a	-> 260a	0.0004	0.0170	-0.0026	-0.0144
9: 252a	-> 260a	0.0003	-0.0247	0.0099	0.0007
9: 258a	-> 264a	0.0003	0.0051	0.0063	-0.0155
9: 258a	-> 274a	0.0002	0.0049	0.0063	-0.0348
9: 256a	-> 260a	0.0002	-0.0114	0.0040	-0.0098
10: 254a	-> 260a	0.9275	1.1029	-0.2573	0.2402
10: 253a	-> 260a	0.0288	-0.2223	0.0134	-0.0164
10: 252a	-> 260a	0.0255	-0.2019	0.0808	0.0059
10: 257a	-> 262a	0.0048	0.0251	-0.0084	0.0020
10: 255a	-> 260a	0.0038	0.0277	-0.0162	0.0268
10: 251a	-> 260a	0.0027	-0.0404	0.0062	0.0342
10: 256a	-> 260a	0.0027	0.0453	-0.0159	0.0387
10: 254a	-> 261a	0.0005	0.0058	-0.0030	-0.0018
10: 257a	-> 260a	0.0004	0.0332	0.0379	0.0117
10: 246a	-> 260a	0.0002	-0.0047	0.0189	0.0019
10: 257a	-> 261a	0.0002	0.0005	0.0016	0.0005
10: 250a	-> 260a	0.0002	-0.0023	0.0007	0.0011
10: 245a	-> 260a	0.0001	0.0063	0.0217	0.0022
10: 253a	-> 264a	0.0001	-0.0159	0.0029	-0.0014
10: 258a	-> 262a	0.0001	0.0012	-0.0036	0.0030
10: 234a	-> 260a	0.0001	-0.0035	-0.0048	-0.0008
10: 248a	-> 260a	0.0001	-0.0067	-0.0013	-0.0034
10: 236a	-> 260a	0.0001	-0.0019	0.0032	-0.0041
10: 252a	-> 264a	0.0001	-0.0123	0.0011	-0.0005
10: 232a	-> 260a	0.0001	-0.0019	0.0021	-0.0012

Table S26 All SINGLET-TRIPLET excitation energies

no.	E/a.u.	E/eV	f	Symmetry
1:	0.02414	0.65678	0.000	A
2:	0.03209	0.87321	0.000	A
3:	0.03935	1.07072	0.000	A
4:	0.05257	1.43042	0.000	A
5:	0.05367	1.46050	0.000	A
6:	0.05540	1.50759	0.000	A
7:	0.05914	1.60930	0.000	A
8:	0.06247	1.69983	0.000	A
9:	0.06358	1.73005	0.000	A
10:	0.06759	1.83922	0.000	A