Supporting Information

A theoretical investigation of thermally activated delayed fluorescent palladium(II) complexes for organic light emitting diodes

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Content

Additional Computational Details

Table S1. TD-DFT Results Calculated at the Geometry Optimized with the Corresponding Functional for Pd1

Table S2. Hole-Electron Analysis of the S_1 State for both Pd(II) Complexes

Table S3. Electronic Transitions of Complex Pd1 Calculated at the T_1 Optimized Geometry by TD-DFT Method. h stands for HOMO, l stands for LUMO

Table S4. Electronic Transitions of Complex Pd2 Calculated at the T_1 Optimized Geometry by TD-DFT Method. h stands for HOMO, l stands for LUMO.

Table S5. Transition Dipole Moments $M_{S_{m,j}}$ (a.u.) for $S_m \rightarrow S_0$ Transitions, Singlet-Triplet Splitting Energies $\Delta E(S_m\text{-}T_1)$ (cm^{-1}), SOCMEs $\left\langle S_m \left| H_{SOC} \right| T_1^{\alpha} \right\rangle$ (cm^{-1}) and k_r^T (s^{-1}) of Complex Pd1.

Table S6. Transition Dipole Moments $M_{S_{m,j}}$ (a.u.) for $S_m \rightarrow S_0$ Transitions, Singlet-Triplet Splitting Energies $\Delta E(S_m\text{-}T_1)$ (cm^{-1}), SOCMEs $\left\langle S_m \left| H_{SOC} \right| T_1^{\alpha} \right\rangle$ (cm^{-1}) and k_r^T (s^{-1}) of Complex Pd2.

Figure S1. Mean Separation Distance (D_{H-L+1}) and the Overlap Extent (S_{H-L+1}) of HOMO and LUMO+1 in the S_0 State for Pd2 (the green region represents HOMO, the blue region represents LUMO+1).

Figure S2. π Electron Density of S_1 State for both Pd(II) Complexes. (a)Pd1, (b)Pd2.

Figure S3. Cele and Chole of S_1 State for both Pd(II) Complexes, Left: Pd1； Right: Pd2. (green region represents electron and blue region represents hole)

Figure S4. Huang-Rhys factor versus frequency of $T_1 \rightarrow S_0$ for both Pd(II) complexes

Optimized Geometries Coordinates of Target Complexes at Different States

Additional Computational Details

1. Functional test

To accurately predict the relative energy between excited states as well as their nature, we compare the results of widely used functionals, PBE0, MN15L, M062X, TPSSh, wB97X-D3 and CAM-B3LYP. For all the functionals, a mixed basis set that includes the 6-311G(d,p) basis set for the C, H, and N atoms, and the SDD pseudo-potential and basis set for the Pd atom were used for the geometry optimization and frequency analysis. The def2-TZVP basis set was used for the energy-related calculations to ensure the accuracy. In all the calculations, a polarizable continuum model was introduced using toluene (η=1.4961) as the solvent and D3 developed by Grimme was introduced. The TD-DFT results calculated at the geometry optimized with the corresponding functional for Pd1 were shown in Table S1. Compared to the experimental results, it is clear that M062X, wB97X-D3 and CAM-B3LYP overestimated the excitation energy while MN15L and TPSSh underestimated the excitation energy, while the PBE0 functional gives ΔE_{ST} =40.5 meV, which is mostly close to the experimental results. So we used PBE0-D3 in this work.

Table S1. TD-DFT Results Calculated at the Geometry Optimized with the Corresponding Functional for Pd1.

Functional	$E(S_1)$\eV	$E(T_1)$\eV
PBE0	1.9348	1.8943
MN15L	1.2248	1.2053
M062X	2.9367	2.7521
TPSSh	1.4052	1.3592
wB97X-D3	3.4186	2.4191
CAM-B3LYP	3.0931	2.2590

2. Basis set used for SOC calculation

In the optimization and frequency calculation by Gaussian, higher level basis was not necessary[1], the 6-311G** for C/H atom and SDD for Pd atom were used to save time. In the energy related calculations, def2-TZVP were used to ensure accuracy. According to the manual for ORCA 5.0.4, ORCA currently does not have SOC integrals for ECPs, and these are by default ignored in the SOC module. In the methodology part, DKH2 represents the use of the popular DKH2 Hamiltonian for scalar relativistic calculations, with the basis set using DKH-def2-TZVP, which is a recontracted version of def2-TZVP specifically designed for DKH calculations. Due to the pseudo-potential basis set of def2-TZVP for Pd, DKH-def2-TZVP is inevitably undefined for Pd. Therefore, SARC-DKH-TZVP is used for Pd element, which is a defined all electron basis set suitable for DKH2 calculation for elements after Xe.

3. Detailed information of the parameters of the equation 1 and equation 3.

$$k_{\mathrm{r}}^{\mathrm{T}_1^{\alpha}}\left(\mathrm{T}_1^{\alpha}\rightarrow \mathrm{S}_0\right)=\frac{8\pi^2\eta^3 E\left(\mathrm{T}_1\right)^3}{3\varepsilon_0\hbar}\sum_{j\in x,y,z}\left|\sum_m \frac{\left\langle \mathrm{S}_m\left|H_{\mathrm{SOC}}\right|\mathrm{T}_1^{\alpha}\right\rangle}{E\left(\mathrm{S}_m\right)-E\left(\mathrm{T}_1\right)}M_{\mathrm{S}_{m.j}}\right|^2 \quad (1)$$

In the equation 1, $E(\mathrm{T}_1)$ is the vertical excitation energy of the T_1 state at S_0 geometry, and $E(\mathrm{S}_m)$ is the vertical excitation energy of the mth singlet excited state at T_1 geometry; $\left\langle \mathrm{S}_m\left|H_{\mathrm{SOC}}\right|\mathrm{T}_1^{\alpha}\right\rangle$ is elements of the SOC matrix between three sublevels (α = I-III) distinguished by the spin quantum number ($\mathrm{M_S}$) of the T_1 state and the coupled S_m state; $M_{\mathrm{S}_{m.j}}$ is the j-axis projection of the $\mathrm{S}_m\rightarrow\mathrm{S}_0$ transition dipole moment.

$$\begin{aligned} k_{\mathrm{nr}}^{\mathrm{T}_1}\left(\mathrm{T}_1\rightarrow \mathrm{S}_0\right)=&\frac{2\pi}{\hbar}\left\langle \mathrm{S}_0\left|H_{\mathrm{SOC}}\right|\mathrm{T}_1\right\rangle^2\left[2\pi\hbar^2\left(D_1^2+P^2\right)\right]^{-1/2}\\ &\times\exp\left[-\frac{\left(\Delta E_{00}-n_{\mathrm{M}}\hbar\omega_{\mathrm{M}}-\lambda_1-\mu\right)^2}{2\pi\hbar^2\left(D_1^2+P^2\right)}\right]\\ &\times\exp\left(-S_{\mathrm{M}}\right)\frac{S_{\mathrm{M}}^{n_{\mathrm{M}}}}{n_{\mathrm{M}}!} \end{aligned} \quad (3)$$

$$\mu=\frac{1}{2}\sum_{j\in\mathrm{lf}}\hbar\omega_j^{\mathrm{S}}\frac{1-b_j}{b_j}\coth\frac{\hbar\omega_j^{\mathrm{T}}}{2k_BT}$$

$$\hbar^2D_1^2=\sum_{j\in\mathrm{lf}}S_j\left(\frac{\hbar\omega_j^{\mathrm{S}}}{b_j}\right)\coth\frac{\hbar\omega_j^{\mathrm{T}}}{2k_BT}$$

$$\hbar^2 P^2 = \frac{1}{2}\sum_{j\in \mathrm{lf}}\left[\hbar\omega_j^{\mathrm{S}}\frac{1-b_j^2}{b_j}\coth\frac{\hbar\omega_j^{\mathrm{T}}}{2k_{\mathrm{B}}T}\right]^2$$

$$\hbar\omega_{\mathrm{M}} = \frac{\lambda_{\mathrm{M}}}{S_{\mathrm{M}}} = \frac{\sum_{j\in \mathrm{hf}} S_j\hbar\omega_j}{\sum_{j\in \mathrm{hf}} S_j}$$

$$\lambda_{\mathrm{l}} = \sum_{j\in \mathrm{lf}}\frac{S_j\hbar\omega_j^{\mathrm{S}}}{b_j}$$

In equation 3, $\omega_j^{\mathrm{S(T)}}$ is the frequency of the *j*th normal mode in the S_0 (T_1) state, hf and lf represent the high-frequency (1000 cm^{-1} < ω_{hf}) and low-frequency (ω_{lf} ≤ 1000 cm^{-1}) regions respectively; $S_j = \frac{1}{2}\omega_j\Delta Q_j^2$ and $\lambda_j = S_j\hbar\omega_j$ are the Huang-Rhys factor and reorganization energy of the *j*th normal mode respectively; $b_j = \omega_j^{\mathrm{T}} / \omega_j^{\mathrm{S}}$ describes the frequency discrepancy in the *j*th normal mode between the T_1 and S_0 states; λ_{l} and λ_{M} are the reorganization energies for the lf and hf regions; $\Delta E'$(= $\Delta E_{00} - \lambda_{\mathrm{l}} - \mu$) represents the effective energy gap between the T_1 and S_0 states affected by the zero-point-energy difference (ΔE_{00}), λ_{l}, and temperature-dependent term (μ); n_{M} =$\Delta E'/\hbar\omega_{\mathrm{M}}$ is the number of vibrational quanta of $\hbar\omega_{\mathrm{M}}$, and it is corrected to the smaller integer of the quotient.

Table S2. Hole-Electron Analysis of the S_1 State for both Pd(II) Complexes

Molecule	Sm(a.u.)	Sr(a.u.)	D(Å)	Contribution of each non-hydrogen atom to hole and electron (Hole: >1%)	
Pd1	0.0382	0.1767	8.314	6(N) Hole: 24.79% Electron: 0.11%	65(C) Hole:5.56% Electron:0.29%
				71(C) Hole: 10.62% Electron: 0.40%	66(C) Hole:4.88% Electron:1.49%
				68(C) Hole: 10.16% Electron: 0.15%	1(Pd) Hole:3.80% Electron:0.59%
				59(C) Hole: 8.92% Electron: 0.04%	60(C) Hole:2.99% Electron:0.08%
				55(C) Hole: 7.50% Electron: 0.00%	64(C) Hole:1.74% Electron:0.72%
				62(C) Hole: 7.00% Electron: 0.12%	63(C) Hole:1.39% Electron:0.11%
Pd2	0.0820	0.2712	7.083	8(N) Hole: 24.68% Electron: 0.02%	13(C) Hole:5.47% Electron:0.05%
				19(C) Hole: 10.58% Electron:-0.05%	11(C) Hole:4.85% Electron:0.29%
				103(C) Hole: 10.04% Electron: 0.04%	1(Pd) Hole:4.22% Electron:0.17%
				107(C) Hole: 9.33% Electron: 0.01%	33(C) Hole:2.99% Electron:0.01%
				105(C) Hole: 7.72% Electron: 0.01%	26(C) Hole:1.48% Electron:0.41%
				32(C) Hole: 7.21% Electron: 0.03%	104(C) Hole:1.45% Electron:0.02%

Table S3. Electronic Transitions of Complex Pd1 Calculated at the T_1 Optimized Geometry by TD-DFT Method. H stands for HOMO, L stands for LUMO

S_n/T_m	Excitation energies (eV)	λ (nm)	f	Main configurations
S_1	1.6587	747.50	0.0897	H → L 99.2%
S_2	2.6380	470.00	0.0177	H → L+1 83.5% H → L+2 10.5%
S_3	2.6914	460.66	0.0569	H-1 → L 50.1% H-2 → L 44.3%
S_4	2.7192	455.96	0.0223	H-2 → L 48.5% H-1 → L 47.7%
S_5	2.8725	431.63	0.0141	H-3 → L 77.4% H → L+2 15.4%
S_6	2.8847	429.80	0.0809	H → L+2 70.0% H-3 → L 17.2% H → L+1 8.5%
S_7	2.9839	415.51	0.0876	H-4 → L 85.8% H-5 → L 7.6%
S_8	3.0400	407.84	0.0454	H-5 → L 84.5% H-4 → L 5.3%
S_9	3.1448	394.25	0.0383	H → L+3 90.3%
S_{10}	3.2810	377.88	0.0047	H-12 → L 80.9% H-11 → L 6.2%

Table S4. Electronic Transitions of Complex Pd2 Calculated at the T_1 Optimized Geometry by TD-DFT Method. H stands for HOMO, L stands for LUMO.

S_n/T_m	Excitation energies (eV)	λ (nm)	f	Main configurations
S_1	2.0192	614.03	0.2574	H → L 97.6%
S_2	2.4393	508.28	0.0025	H → L+1 99.1%
S_3	3.0159	411.11	0.0168	H-2 → L 81.4% H → L+2 9.2%
S_4	3.0371	408.23	0.0331	H → L+2 60.2% H → L+3 25.8% H-2 → L 11.1%
S_5	3.0684	404.07	0.0134	H-1 → L 92.5%
S_6	3.1935	388.24	0.0341	H → L+3 59.6% H → L+2 21.7% H → L+5 9.7%
S_7	3.3124	374.31	0.0196	H-3 → L+1 97.0%
S_8	3.3655	368.39	0.0003	H → L+4 96.3%
S_9	3.4348	360.97	0.0007	H-2 → L+1 83.0% H-1 → L+1 7.8%
S_{10}	3.4464	359.75	0.0043	H-4 → L 90.5%

Table S5. Transition Dipole Moments $M_{S_{m,j}}$ (a.u.) for $S_m \rightarrow S_0$ Transitions, Singlet-Triplet Splitting Energies $|\Delta E(S_m\text{-}T_1)|$ (cm^{-1}), SOCMEs $\left\langle S_m \left| H_{SOC} \right| T_1^{\alpha} \right\rangle$ (cm^{-1}) and k_r^T (s^{-1}) of Complex Pd1.

S_m	$\lvert\Delta E(S_m\text{-}T_1)\rvert$	$M_{S_{m,x}}$	$M_{S_{m,y}}$	$M_{S_{m,z}}$	$\left\langle S_m \left\lvert H_{SOC} \right\rvert T_1^{I} \right\rangle$	$\left\langle S_m \left\lvert H_{SOC} \right\rvert T_1^{II} \right\rangle$	$\left\langle S_m \left\lvert H_{SOC} \right\rvert T_1^{III} \right\rangle$
S_1	1900.24	-1.4764	-0.1566	0.0645	1.29	3.62	3.62
S_2	5998.34	-0.5167	-0.0118	-0.0780	1.60	0.95	0.95
S_3	6429.04	-0.9000	0.1472	0.1777	14.76	16.27	16.27
S_4	6653.26	-0.5775	0.0111	0.0238	16.87	19.48	19.48
S_5	7889.71	0.1644	0.3377	-0.2432	7.71	33.48	33.48
S_6	7988.11	1.0531	0.1900	0.0160	0.92	1.10	1.10
S_7	8788.21	0.8877	0.4027	-0.4981	19	55.46	55.46
S_8	9240.69	-0.6953	-0.1816	0.3050	11.86	32.08	32.08
S_9	10085.96	-0.6700	0.2202	-0.0143	5.56	4.32	4.32
S_{10}	11184.48	-0.2137	-0.0927	-0.0610	0.5	4.13	4.13
k_r^T	3994.82						

Table S6. Transition Dipole Moments $M_{S_{m,j}}$ (a.u.) for $S_m \rightarrow S_0$ Transitions, Singlet-Triplet Splitting Energies $|\Delta E(S_m\text{-}T_1)|$ (cm^{-1}), SOCMEs $\left\langle S_m \left| H_{SOC} \right| T_1^{\alpha} \right\rangle$ (cm^{-1}) and k_r^T (s^{-1}) of Complex Pd2.

S_m	$\Delta E(S_m\text{-}T_1)$	$M_{S_{m,x}}$	$M_{S_{m,y}}$	$M_{S_{m,z}}$	$\left\langle S_m \left| H_{SOC} \right| T_1^{I} \right\rangle$	$\left\langle S_m \left| H_{SOC} \right| T_1^{II} \right\rangle$	$\left\langle S_m \left| H_{SOC} \right| T_1^{III} \right\rangle$
S_1	1433.15	2.2757	-0.0123	0.1535	0.32	4.38	4.38
S_2	1954.96	0.2031	-0.0230	0.0134	-0.54	0.91	0.91
S_3	6605.24	0.2321	0.3638	-0.2039	15.28	27.14	27.14
S_4	6776.21	0.6058	0.2752	-0.0512	9.33	10.17	10.17
S_5	7028.65	0.0780	0.3300	-0.2523	3.64	1.95	1.95
S_6	8037.58	-0.6532	-0.0417	-0.0881	2.99	2.70	2.70
S_7	8996.51	-0.4468	0.1080	-0.1726	2.61	34.32	34.32
S_8	9424.76	0.0097	-0.0597	0.0192	10.8	12.60	12.60
S_9	9983.66	0.0263	-0.0532	0.0701	-3.71	66.75	66.75
S_{10}	10077.22	0.2041	-0.0386	-0.0874	-0.64	5.72	5.72
k_r^T	4420.28						

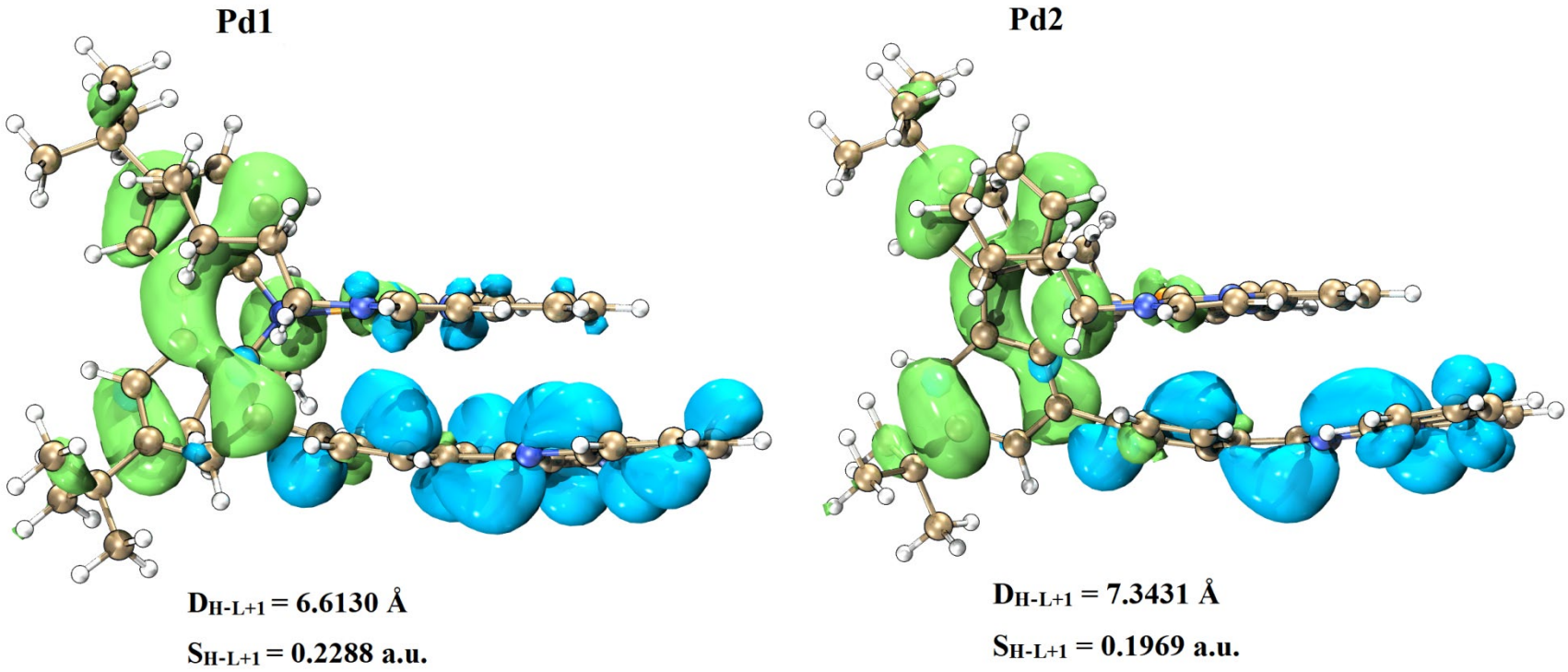
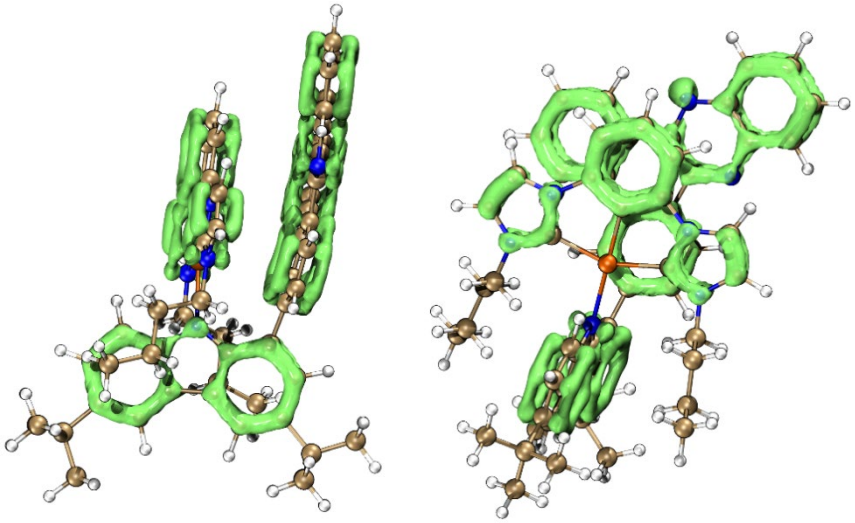
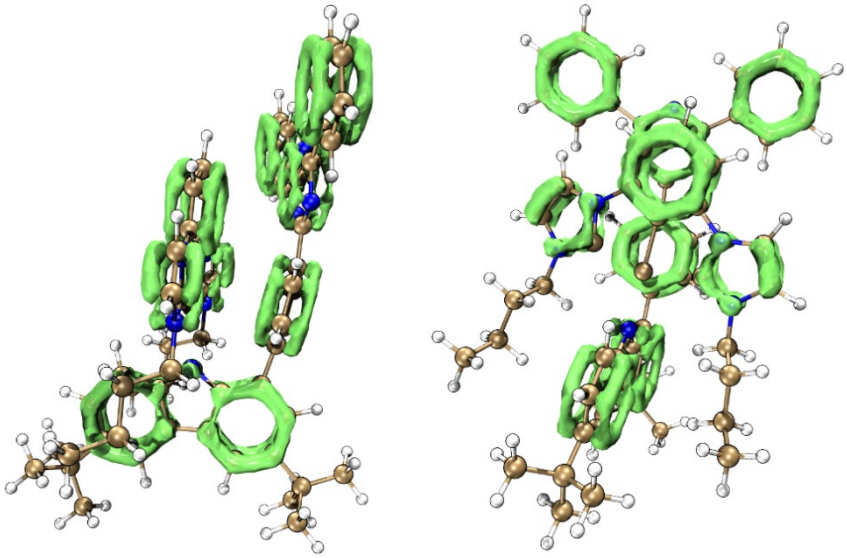


Figure S1. Mean Separation Distance (D_{H-L+1}) and the Overlap Extent (S_{H-L+1}) of HOMO and LUMO+1 at the S_0 State for Target Complexes (the green region represents HOMO, the blue region represents LUMO+1)



(a)Pd1



(b)Pd2

Figure S2. π Electron Density of S_1 State for both Pd(II) Complexes. (a)Pd1, (b)Pd2.

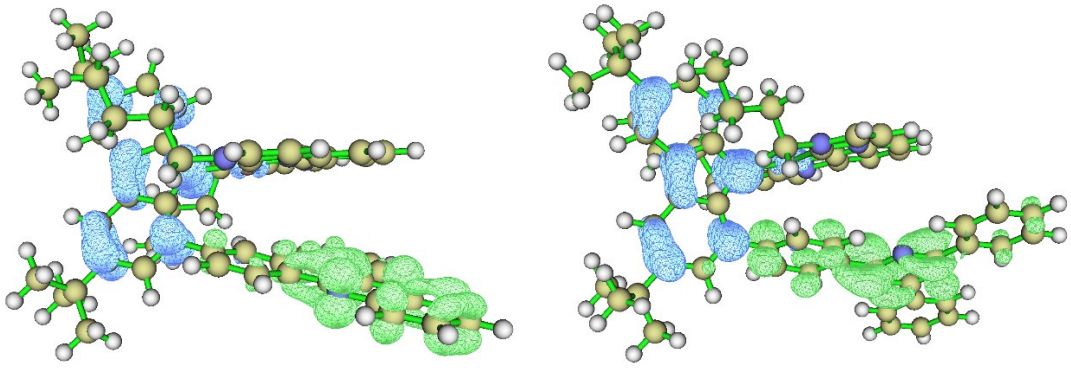


Figure S3. Cele and Chole of S_1 State for both Pd(II) Complexes, Left: Pd1； Right: Pd2. (green region represents electron and blue region represents hole)

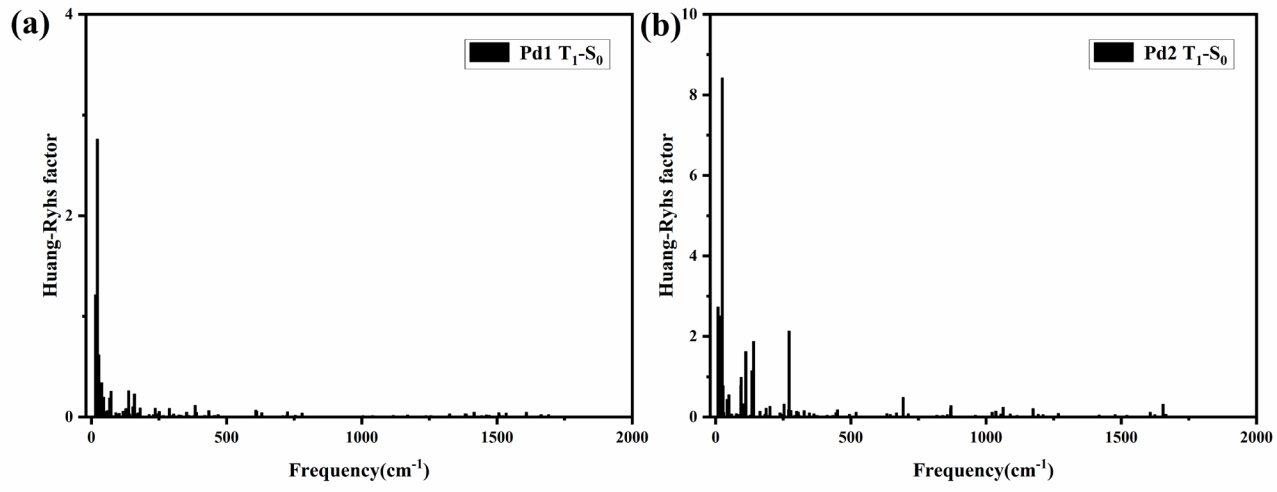


Figure S4. Huang-Rhys factor versus frequency of $T_1 \rightarrow S_0$ for both Pd(II) complexes

Optimized Geometries Coordinates of Target Complexes at Different States

Pd1(CCDC:2218304)

S_0 geometry optimized at PBE0(D3BJ)/6-311G(d,p)+SDD(Pd) with toluene as solvent

46	0.207060	-0.822300	-0.649636
7	1.542012	-3.144793	0.454105
7	-0.398270	-3.284116	1.353483
7	2.176754	0.429865	-2.358684
7	0.459742	1.680854	-2.633437
7	4.833357	2.089390	-0.384668
7	6.109837	-0.122500	0.778953
7	-1.748048	-0.128319	-0.235909
6	4.865422	0.187527	1.081509
6	6.744980	0.642847	-0.127674
6	-4.244994	2.113832	1.109579
1	-5.330974	2.149560	1.108455
6	-3.599748	1.056028	0.478781
6	-0.897349	2.207699	-2.568973
1	-0.862863	3.236665	-2.936385
1	-1.194141	2.234079	-1.519777
6	4.108531	-2.562857	3.504838
1	4.618752	-3.396791	3.974937
6	-1.422220	1.977237	1.104980
6	4.785657	-1.739722	2.629644
1	5.828145	-1.907805	2.388234
6	0.815848	2.884309	0.407312
1	0.313975	3.722441	-0.065151
6	-2.109942	3.028553	1.706718
1	-1.513347	3.794142	2.189650
6	-2.173041	0.968532	0.468695
6	2.524825	-2.552939	-0.374330
6	2.764191	-2.309721	3.788221
1	2.223315	-2.947211	4.479259
6	0.056036	1.933102	1.103619
6	6.095161	1.763546	-0.721303
6	-4.058499	-0.082180	-0.268787
6	-5.318090	-0.573525	-0.618871
1	-6.203547	-0.039725	-0.291409
6	2.115906	-1.247435	3.190960
1	1.076339	-1.068528	3.432857
6	2.103073	0.713695	1.633311
6	4.139131	-0.656804	2.020505
6	2.781970	-0.400457	2.291579
6	0.866614	0.578280	-1.985279

6	0.318799	-2.525011	0.504270
6	0.719262	0.891136	1.737194
1	0.127631	0.194157	2.313106
6	2.824208	1.603011	0.814747
6	4.213819	1.323024	0.492590
6	2.027018	-1.428841	-1.006305
6	-4.328274	0.980423	-3.876546
1	-5.342537	1.373877	-3.764190
1	-4.307936	-0.015043	-3.424351
1	-4.126304	0.873981	-4.947993
6	-3.454287	-0.280410	3.914082
1	-3.064002	0.585187	3.370441
1	-2.891076	-0.379425	4.848524
1	-4.494693	-0.064819	4.172334
6	-3.343142	-1.539678	3.066593
1	-3.917710	-1.405899	2.143127
1	-3.787435	-2.392643	3.595579
6	-1.899158	-1.853544	2.703291
1	-1.465875	-0.978640	2.213545
1	-1.312831	-2.060036	3.608389
6	-5.138043	4.996953	1.429491
1	-5.878149	4.325947	0.985878
1	-4.539030	5.418672	0.616826
1	-5.676686	5.815032	1.919979
6	4.647626	-2.208515	-1.406905
1	5.679328	-2.506496	-1.553303
6	-5.111896	3.691202	3.565681
1	-5.651581	4.493816	4.080214
1	-4.493371	3.166348	4.299770
1	-5.848866	2.981058	3.181313
6	-1.781114	-3.019789	1.739298
1	-2.171563	-3.940657	2.180003
1	-2.349744	-2.815145	0.830625
6	4.179118	-1.061380	-2.050536
1	4.841329	-0.483113	-2.685593
6	-3.280302	5.282404	3.046938
1	-2.642639	5.741726	2.285532
1	-2.636426	4.827748	3.805622
1	-3.850885	6.081191	3.530075
6	-3.307064	1.888180	-3.208514
1	-3.540539	1.966343	-2.140662
1	-3.376030	2.903438	-3.620790
6	1.485816	2.223299	-3.385640
1	1.353562	3.117401	-3.971768

6	1.578992	-4.255371	1.260872
1	2.451975	-4.875575	1.369830
6	2.574517	1.435261	-3.208164
1	3.574348	1.514483	-3.599271
6	2.859802	-0.689033	-1.829777
6	3.837566	-2.967471	-0.561973
1	4.240938	-3.839062	-0.059084
6	-4.242609	4.263389	2.437211
6	0.352805	-4.343125	1.830856
1	-0.050938	-5.063117	2.523017
6	8.069242	0.325244	-0.512080
1	8.541587	-0.531312	-0.044107
6	2.174008	2.707627	0.249725
1	2.759879	3.390201	-0.353937
6	6.787352	2.534933	-1.685281
1	6.272754	3.385043	-2.119541
6	8.066431	2.199679	-2.041541
1	8.595850	2.790487	-2.781248
6	-3.511179	3.119460	1.735234
6	-2.878760	-0.755808	-0.684044
6	-2.985419	-1.915034	-1.463629
1	-2.090517	-2.429923	-1.801822
6	-5.433222	-1.729405	-1.381249
6	-1.884152	1.370130	-3.363043
1	-1.829830	0.340630	-2.995918
1	-1.593077	1.356311	-4.420916
6	-4.246666	-2.378628	-1.790581
1	-4.320461	-3.277547	-2.395281
6	8.712222	1.087210	-1.450722
1	9.726154	0.841714	-1.747385
6	-6.920229	-3.737460	-1.255920
1	-6.126291	-4.389946	-1.628806
1	-7.880528	-4.171440	-1.555146
1	-6.868740	-3.737206	-0.162945
6	-6.869491	-2.342676	-3.335297
1	-6.779105	-1.333437	-3.747670
1	-7.830056	-2.761111	-3.655141
1	-6.074913	-2.953850	-3.771334
6	-7.954794	-1.483517	-1.277971
1	-7.962055	-1.442118	-0.184588
1	-8.896838	-1.936517	-1.601196
1	-7.928927	-0.458860	-1.660793
6	-6.781468	-2.310010	-1.802927

S_1 geometry optimized at PBE0(D3BJ)/6-311G(d,p)+SDD(Pd) with toluene as solvent

46	0.169409	-0.857420	-0.614766
7	1.414374	-3.212501	0.537427
7	-0.549644	-3.304202	1.382471
7	2.237572	0.345281	-2.249553
7	0.572185	1.645891	-2.582964
7	4.756309	2.132126	-0.480404
7	6.179432	-0.036008	0.700079
7	-1.779947	-0.109916	-0.252735
6	4.910047	0.255178	1.033316
6	6.743246	0.743006	-0.257370
6	-4.255994	2.069164	1.187635
1	-5.338277	2.137633	1.171945
6	-3.618072	1.060680	0.505660
6	-0.762082	2.221125	-2.558745
1	-0.676291	3.259395	-2.887942
1	-1.096586	2.233517	-1.520883
6	4.317759	-2.533640	3.453544
1	4.879596	-3.343080	3.909488
6	-1.418001	1.888453	1.217807
6	4.938022	-1.668062	2.581459
1	5.983636	-1.774533	2.318892
6	0.781927	2.815393	0.473267
1	0.255622	3.655152	0.029773
6	-2.102085	2.902550	1.893182
1	-1.500873	3.621895	2.433977
6	-2.198857	0.953668	0.517177
6	2.434478	-2.645672	-0.262520
6	2.959407	-2.362324	3.757542
1	2.462770	-3.037320	4.446838
6	0.060994	1.843656	1.192381
6	6.025138	1.831181	-0.856763
6	-4.082731	-0.029462	-0.339232
6	-5.324484	-0.474168	-0.747694
1	-6.218510	0.038958	-0.416251
6	2.253947	-1.327085	3.182351
1	1.207720	-1.205808	3.438650
6	2.139907	0.659150	1.662443
6	4.234314	-0.606817	1.982994
6	2.863604	-0.428820	2.287833
6	0.920349	0.520878	-1.938843
6	0.209302	-2.569364	0.546676
6	0.748942	0.809706	1.798849

1	0.191206	0.093463	2.387624
6	2.828795	1.562921	0.821576
6	4.210696	1.334703	0.456722
6	1.983190	-1.518676	-0.920338
6	-4.189234	1.182463	-4.042165
1	-5.195938	1.592884	-3.923784
1	-4.205306	0.150113	-3.681328
1	-3.961387	1.159982	-5.112568
6	-3.575550	-0.324778	4.010843
1	-3.112842	0.554492	3.552809
1	-3.066770	-0.513981	4.961292
1	-4.616403	-0.074396	4.232766
6	-3.478196	-1.529008	3.086139
1	-4.013968	-1.316942	2.153151
1	-3.978942	-2.393057	3.540106
6	-2.035281	-1.885811	2.760681
1	-1.530364	-1.005269	2.355184
1	-1.498800	-2.171579	3.673373
6	-5.059222	4.942391	1.687185
1	-5.806982	4.330992	1.175512
1	-4.424559	5.407630	0.927676
1	-5.587158	5.735573	2.224981
6	4.606454	-2.338569	-1.194990
1	5.643610	-2.639236	-1.277773
6	-5.136046	3.471685	3.718903
1	-5.665860	4.249329	4.277219
1	-4.556882	2.873822	4.428052
1	-5.884191	2.820133	3.259870
6	-1.929278	-3.002730	1.737394
1	-2.375596	-3.925706	2.115536
1	-2.459237	-2.733900	0.822868
6	4.186189	-1.187641	-1.860280
1	4.892178	-0.603544	-2.439096
6	-3.251085	5.057364	3.388981
1	-2.582528	5.566137	2.688691
1	-2.641312	4.527705	4.126323
1	-3.821198	5.824375	3.919742
6	-3.162407	2.003908	-3.277943
1	-3.431469	2.025522	-2.214902
1	-3.186565	3.045808	-3.620762
6	1.651627	2.177918	-3.267368
1	1.577181	3.094548	-3.827820
6	1.409631	-4.310347	1.360163
1	2.270987	-4.939011	1.505253

6	2.708253	1.358554	-3.047777
1	3.737493	1.433726	-3.353499
6	2.866583	-0.793978	-1.701113
6	3.746304	-3.081311	-0.388358
1	4.114065	-3.947553	0.148971
6	-4.216686	4.116440	2.670475
6	0.167141	-4.370410	1.896478
1	-0.268123	-5.070842	2.589470
6	8.053271	0.476685	-0.696225
1	8.578407	-0.348742	-0.226327
6	2.134005	2.661639	0.281110
1	2.701521	3.358798	-0.323436
6	6.655469	2.584935	-1.864605
1	6.095610	3.407918	-2.298088
6	7.947640	2.294466	-2.278291
1	8.414729	2.891640	-3.054930
6	-3.494603	3.015516	1.905214
6	-2.904866	-0.691337	-0.768169
6	-2.982124	-1.801072	-1.615723
1	-2.076217	-2.298395	-1.945837
6	-5.420010	-1.589646	-1.595397
6	-1.750087	1.454173	-3.420833
1	-1.729063	0.402320	-3.118071
1	-1.431125	1.489321	-4.469152
6	-4.235687	-2.231082	-2.009482
1	-4.303177	-3.089686	-2.667376
6	8.648448	1.238129	-1.691367
1	9.660426	1.012828	-2.012389
6	-6.924301	-3.577344	-1.639738
1	-6.135677	-4.217922	-2.041817
1	-7.884529	-3.969004	-1.988499
1	-6.899486	-3.653299	-0.548827
6	-6.792723	-2.046060	-3.623595
1	-6.674082	-1.014682	-3.967299
1	-7.750816	-2.423088	-3.993772
1	-5.999052	-2.645738	-4.075720
6	-7.939639	-1.311388	-1.545896
1	-7.986136	-1.344554	-0.453332
1	-8.872938	-1.732019	-1.928954
1	-7.895597	-0.264617	-1.861026
6	-6.760875	-2.117988	-2.089421

T_1 geometry optimized at PBE0(D3BJ)/6-311G(d,p)+SDD(Pd) with toluene as solvent

46	0.147335	-0.855677	-0.641243
7	1.374032	-3.325897	0.267009
7	-0.563220	-3.455276	1.169141
7	2.218850	0.476079	-2.170877
7	0.551609	1.794482	-2.417162
7	4.845725	2.191833	-0.270443
7	6.159379	-0.152986	0.682902
7	-1.782180	-0.131295	-0.187787
6	4.901965	0.136805	1.016112
6	6.777536	0.715282	-0.168331
6	-4.206770	2.136024	1.181156
1	-5.288052	2.222053	1.169827
6	-3.595574	1.064426	0.579485
6	-0.784861	2.366092	-2.366901
1	-0.706207	3.401832	-2.705386
1	-1.101083	2.385871	-1.323386
6	4.184485	-2.846810	3.158607
1	4.714979	-3.707931	3.552860
6	-1.366852	1.914087	1.199393
6	4.845339	-1.925788	2.376735
1	5.893371	-2.039352	2.126507
6	0.872582	2.892517	0.690113
1	0.383964	3.803674	0.357940
6	-2.035779	3.017929	1.760819
1	-1.418442	3.773185	2.230628
6	-2.173779	0.935521	0.576862
6	2.393598	-2.696180	-0.484434
6	2.826685	-2.662226	3.452946
1	2.299577	-3.377674	4.075567
6	0.089177	1.835146	1.211537
6	6.111947	1.889928	-0.646907
6	-4.088562	-0.041039	-0.223932
6	-5.348438	-0.471774	-0.606420
1	-6.227233	0.057483	-0.258639
6	2.158365	-1.563811	2.955802
1	1.112396	-1.431039	3.207156
6	2.127551	0.544857	1.609138
6	4.181159	-0.798135	1.864213
6	2.810061	-0.611911	2.151356
6	0.899368	0.626776	-1.852375
6	0.180889	-2.666103	0.368171
6	0.740308	0.693206	1.678493
1	0.145847	-0.074092	2.155996
6	2.873171	1.529519	0.906165

6	4.241417	1.304109	0.552319
6	1.951783	-1.505631	-1.026905
6	-4.233738	1.293413	-3.773962
1	-5.241150	1.697762	-3.641448
1	-4.235700	0.265927	-3.398834
1	-4.025846	1.258970	-4.848268
6	-3.453605	-0.491771	3.964265
1	-3.016116	0.386799	3.480037
1	-2.896516	-0.677481	4.888044
1	-4.481948	-0.241498	4.238480
6	-3.403967	-1.699258	3.039150
1	-3.981367	-1.487043	2.131391
1	-3.886016	-2.560202	3.518591
6	-1.978794	-2.061299	2.646656
1	-1.492002	-1.177479	2.227807
1	-1.402847	-2.359317	3.531032
6	-4.992121	5.044211	1.431888
1	-5.755749	4.389114	1.004925
1	-4.380514	5.430711	0.611575
1	-5.503336	5.888244	1.904957
6	4.571365	-2.311154	-1.375902
1	5.606453	-2.609859	-1.487768
6	-5.007434	3.775847	3.597013
1	-5.523294	4.602720	4.094855
1	-4.405843	3.247705	4.342265
1	-5.766337	3.083211	3.223608
6	-1.923439	-3.164929	1.605030
1	-2.340013	-4.095643	1.997390
1	-2.508717	-2.888418	0.727117
6	4.160896	-1.094714	-1.920544
1	4.872686	-0.461126	-2.437473
6	-3.135096	5.320327	3.058653
1	-2.484435	5.751211	2.292082
1	-2.506905	4.866281	3.830209
1	-3.689578	6.140482	3.522597
6	-3.199018	2.132041	-3.039331
1	-3.446064	2.160412	-1.971241
1	-3.239164	3.170506	-3.391570
6	1.631634	2.374231	-3.059207
1	1.556269	3.327555	-3.554505
6	1.374687	-4.488686	0.994844
1	2.227511	-5.142159	1.057462
6	2.689194	1.543195	-2.896790
1	3.717081	1.638659	-3.201155

6	2.841852	-0.711833	-1.729400
6	3.702819	-3.126573	-0.652201
1	4.062906	-4.046428	-0.206389
6	-4.120310	4.315055	2.464961
6	0.149314	-4.572581	1.565868
1	-0.277288	-5.322527	2.210803
6	8.085378	0.451795	-0.602528
1	8.567971	-0.443447	-0.222918
6	2.218224	2.720822	0.503808
1	2.822033	3.475214	0.014301
6	6.797388	2.737548	-1.540646
1	6.276112	3.624812	-1.886970
6	8.087542	2.449882	-1.953921
1	8.597015	3.117678	-2.641645
6	-3.419520	3.143230	1.789592
6	-2.931871	-0.716600	-0.674328
6	-3.039169	-1.818414	-1.522919
1	-2.147380	-2.322146	-1.882090
6	-5.476471	-1.585126	-1.444944
6	-1.786051	1.591085	-3.206583
1	-1.754825	0.540861	-2.900003
1	-1.486358	1.624064	-4.260826
6	-4.308205	-2.236511	-1.886813
1	-4.398414	-3.092836	-2.545850
6	8.735575	1.303826	-1.483811
1	9.747486	1.080483	-1.806346
6	-7.002452	-3.560311	-1.464429
1	-6.228067	-4.205869	-1.886158
1	-7.973468	-3.943423	-1.793273
1	-6.953770	-3.641039	-0.374573
6	-6.903041	-2.020067	-3.442332
1	-6.779569	-0.987805	-3.782251
1	-7.873448	-2.384058	-3.794037
1	-6.125917	-2.625289	-3.915714
6	-7.991918	-1.286479	-1.333970
1	-8.008078	-1.321569	-0.240500
1	-8.939125	-1.698303	-1.692472
1	-7.947135	-0.239291	-1.647645
6	-6.834275	-2.100787	-1.910211

Pd2(CCDC:2226102)

S_0 geometry optimized at PBE0(D3BJ)/6-311G(d,p)+SDD(Pd) with toluene as solvent

46	-0.180235	0.572516	-0.557310

7	0.032778	-2.389526	-1.771663
7	1.735971	-1.101448	-1.934961
7	1.235673	3.045420	-0.032217
7	-0.633874	3.349741	0.971975
7	-2.155417	0.079336	0.056946
7	4.257858	0.405064	1.551549
7	6.203723	-0.194923	0.360428
7	4.421263	-1.729214	0.560877
6	-4.769301	-2.193414	-3.119808
1	-4.772805	-1.108040	-2.987572
1	-5.775675	-2.557696	-2.894280
1	-4.563112	-2.408928	-4.173920
6	-3.732052	-2.834434	-2.211160
1	-3.768833	-3.927595	-2.306613
1	-3.972939	-2.601688	-1.167939
6	-2.323947	-2.342646	-2.513047
1	-2.300889	-1.249317	-2.464328
1	-2.028722	-2.630271	-3.530056
6	-1.314286	-2.882533	-1.515939
1	-1.591614	-2.584202	-0.504027
1	-1.270625	-3.974469	-1.546019
6	1.042699	-3.121048	-2.369769
1	0.904959	-4.146604	-2.669537
6	2.123638	-2.308401	-2.467644
1	3.111898	-2.492164	-2.853947
6	0.439574	-1.141349	-1.490763
6	2.435145	0.111480	-1.739273
6	1.636098	1.042749	-1.099657
6	2.172327	2.273031	-0.760558
6	3.479751	2.610182	-1.084496
1	3.913411	3.565713	-0.811717
6	4.250353	1.658926	-1.754928
1	5.278151	1.897078	-2.003396
6	3.750221	0.397926	-2.083429
1	4.385991	-0.328169	-2.578460
6	0.010570	2.470739	0.187935
6	1.341556	4.258373	0.608765
1	2.229027	4.867560	0.572171
6	0.156884	4.454101	1.238810
1	-0.187033	5.273622	1.847670
6	-1.997277	3.158242	1.447688
1	-2.006218	3.318012	2.530435
1	-2.240217	2.112705	1.251252
6	-2.988809	4.077076	0.754908

1	-2.759497	5.123338	0.995515
1	-2.874138	3.961757	-0.328264
6	-4.422906	3.753351	1.148347
1	-4.660108	2.737615	0.812363
1	-4.512113	3.751737	2.242332
6	-5.418177	4.737431	0.554867
1	-6.444451	4.480462	0.830459
1	-5.359038	4.737302	-0.537449
1	-5.223929	5.757929	0.901859
6	-3.374465	1.430585	-1.655608
1	-2.476550	1.866396	-2.083979
6	-4.627179	1.729201	-2.160252
1	-4.690329	2.416348	-2.998828
6	-5.817627	1.167991	-1.644291
6	-5.714904	0.287231	-0.574804
1	-6.601882	-0.172713	-0.153167
6	-4.463782	-0.032552	-0.041394
6	-3.279325	0.535917	-0.582491
6	-2.594633	-0.798394	1.014903
6	-4.017356	-0.920482	0.996734
6	-4.664092	-1.824220	1.833664
1	-5.747195	-1.902606	1.794037
6	-3.934413	-2.638179	2.698123
6	-2.536426	-2.502108	2.710650
1	-1.943945	-3.109426	3.385527
6	-1.850819	-1.592172	1.910235
6	-7.151855	1.508633	-2.307209
6	-8.329934	0.824615	-1.614573
1	-8.243019	-0.265367	-1.652810
1	-9.262084	1.102001	-2.115886
1	-8.411131	1.126844	-0.566041
6	-7.390968	3.023199	-2.265197
1	-7.446741	3.376578	-1.232203
1	-8.332042	3.274800	-2.766221
1	-6.588722	3.572954	-2.764596
6	-7.123444	1.043643	-3.770441
1	-6.318886	1.528411	-4.329795
1	-8.070704	1.282392	-4.266307
1	-6.967007	-0.037287	-3.828874
6	-4.666129	-3.640986	3.590662
6	-3.708330	-4.443442	4.471028
1	-2.999222	-5.023694	3.872928
1	-4.278249	-5.146269	5.086088
1	-3.139711	-3.795915	5.145094

6	-5.447120	-4.628322	2.712059
1	-6.181581	-4.114122	2.086657
1	-5.982368	-5.354947	3.333046
1	-4.768843	-5.175225	2.050217
6	-5.645423	-2.894908	4.506970
1	-5.110928	-2.187267	5.147519
1	-6.184303	-3.600626	5.148585
1	-6.384480	-2.332243	3.930633
6	-0.381235	-1.471708	1.954305
6	0.449916	-2.533349	1.583700
1	0.005194	-3.496708	1.355468
6	1.809633	-2.338526	1.410291
1	2.441887	-3.137320	1.041500
6	2.375655	-1.082943	1.644705
6	1.571049	-0.053967	2.136942
1	2.019477	0.911779	2.334500
6	0.208006	-0.244144	2.276439
1	-0.425159	0.572120	2.605745
6	3.761215	-0.797746	1.254985
6	5.631470	-1.377762	0.130982
6	5.471654	0.664440	1.072811
6	6.367781	-2.351314	-0.699953
6	5.768483	-3.561944	-1.056820
1	4.768488	-3.771811	-0.696474
6	6.448179	-4.466762	-1.858829
1	5.978356	-5.405432	-2.132661
6	7.731505	-4.172876	-2.309522
1	8.262705	-4.881804	-2.935863
6	8.333039	-2.969348	-1.955620
1	9.333917	-2.739483	-2.304837
6	7.654985	-2.060886	-1.156099
1	8.106657	-1.117791	-0.873350
6	6.023467	2.012120	1.312922
6	7.273182	2.365726	0.802396
1	7.839765	1.623722	0.252988
6	7.768049	3.647824	0.994049
1	8.739472	3.917243	0.593607
6	7.020614	4.586228	1.698234
1	7.408794	5.588336	1.847446
6	5.775542	4.236955	2.213366
1	5.192950	4.965688	2.767149
6	5.277788	2.956882	2.021723
1	4.308026	2.668284	2.408603

S_1 geometry optimized at PBE0(D3BJ)/6-311G(d,p)+SDD(Pd) with toluene as solvent

46	-0.129530	0.482640	-0.543982
7	0.043392	-2.570358	-1.533810
7	1.760228	-1.322773	-1.799537
7	1.359738	2.944337	-0.155648
7	-0.492791	3.367372	0.830603
7	-2.141578	0.081307	0.035062
7	4.251096	0.429188	1.690210
7	6.118590	-0.256711	0.388997
7	4.272473	-1.739617	0.718476
6	-4.741787	-2.560047	-2.966959
1	-4.718959	-1.468705	-3.033832
1	-5.756609	-2.856794	-2.687482
1	-4.538968	-2.960894	-3.965074
6	-3.718946	-3.054892	-1.956497
1	-3.768528	-4.147924	-1.877196
1	-3.968791	-2.663873	-0.962939
6	-2.301427	-2.633407	-2.316136
1	-2.259219	-1.546666	-2.443992
1	-2.004665	-3.077130	-3.273757
6	-1.304115	-3.028521	-1.240784
1	-1.594944	-2.604125	-0.279433
1	-1.262646	-4.114108	-1.122089
6	1.052143	-3.365821	-2.050388
1	0.909018	-4.415264	-2.246239
6	2.142239	-2.576398	-2.209893
1	3.143560	-2.808863	-2.533112
6	0.466232	-1.306267	-1.365695
6	2.479537	-0.111580	-1.689349
6	1.703099	0.873001	-1.107512
6	2.270102	2.105453	-0.843251
6	3.582464	2.391832	-1.190483
1	4.043364	3.345138	-0.959201
6	4.326305	1.387419	-1.807731
1	5.362463	1.579723	-2.057650
6	3.795728	0.122505	-2.059311
1	4.417763	-0.655858	-2.485547
6	0.121716	2.425553	0.092959
6	1.511975	4.182701	0.420306
1	2.426191	4.748669	0.360947
6	0.336816	4.455831	1.038492
1	0.024221	5.316046	1.606762
6	-1.865741	3.273596	1.297593

1	-1.900839	3.642490	2.326657
1	-2.117713	2.213316	1.314957
6	-2.832176	4.040786	0.410945
1	-2.589093	5.109744	0.442790
1	-2.691026	3.714546	-0.625352
6	-4.280261	3.822486	0.823583
1	-4.522480	2.757879	0.725658
1	-4.401595	4.072663	1.884938
6	-5.247654	4.644961	-0.012475
1	-6.285231	4.455409	0.275520
1	-5.146059	4.401308	-1.073887
1	-5.059315	5.716795	0.104372
6	-3.215365	1.234991	-1.886687
1	-2.277615	1.572132	-2.314968
6	-4.431443	1.511558	-2.485672
1	-4.433602	2.082489	-3.406979
6	-5.656583	1.062811	-1.954930
6	-5.644063	0.324817	-0.759559
1	-6.570353	-0.034139	-0.328930
6	-4.442096	0.041929	-0.141960
6	-3.219593	0.488347	-0.704858
6	-2.641632	-0.630829	1.101703
6	-4.061607	-0.706194	1.046802
6	-4.763517	-1.435224	1.976929
1	-5.844821	-1.495360	1.918253
6	-4.069257	-2.121666	2.996469
6	-2.675414	-2.030733	3.038064
1	-2.126350	-2.543339	3.817193
6	-1.930683	-1.289817	2.118710
6	-6.948261	1.352660	-2.711596
6	-8.178402	0.800127	-1.992516
1	-8.133721	-0.287941	-1.887705
1	-9.073630	1.038425	-2.572606
1	-8.300889	1.241722	-0.998966
6	-7.126252	2.868334	-2.873634
1	-7.215990	3.356450	-1.900086
1	-8.036090	3.074619	-3.445063
1	-6.287687	3.324219	-3.405788
6	-6.866172	0.698620	-4.099719
1	-6.027284	1.086807	-4.682499
1	-7.785173	0.898951	-4.658622
1	-6.746493	-0.384819	-4.014721
6	-4.862360	-2.938235	4.008107
6	-3.965532	-3.615077	5.043315

1	-3.262704	-4.312295	4.578367
1	-4.584922	-4.185232	5.740572
1	-3.395568	-2.885930	5.626067
6	-5.648513	-4.026584	3.261400
1	-6.350547	-3.601011	2.539760
1	-6.223271	-4.625386	3.974187
1	-4.970613	-4.694055	2.721821
6	-5.841367	-2.011958	4.744513
1	-5.303225	-1.224628	5.279728
1	-6.420339	-2.587247	5.473089
1	-6.546778	-1.535049	4.059161
6	-0.455716	-1.225331	2.170956
6	0.316536	-2.346150	1.851868
1	-0.171720	-3.300232	1.678002
6	1.684592	-2.222961	1.672642
1	2.283235	-3.063891	1.343170
6	2.311882	-0.988423	1.839906
6	1.561356	0.095768	2.290335
1	2.068325	1.040487	2.443012
6	0.185308	-0.015324	2.431913
1	-0.403380	0.849645	2.720063
6	3.717806	-0.778522	1.414262
6	5.500941	-1.456033	0.182321
6	5.467533	0.617850	1.117951
6	6.100438	-2.410621	-0.702029
6	5.466275	-3.645330	-0.990035
1	4.530570	-3.867040	-0.490802
6	6.028026	-4.545594	-1.876545
1	5.519945	-5.486012	-2.072900
6	7.239639	-4.267632	-2.515458
1	7.676357	-4.977430	-3.208994
6	7.879945	-3.056085	-2.235015
1	8.825164	-2.823641	-2.717589
6	7.331078	-2.146656	-1.351920
1	7.830750	-1.209197	-1.138981
6	6.068330	1.959039	1.284701
6	7.309551	2.266425	0.720965
1	7.836035	1.483596	0.187526
6	7.842466	3.540971	0.840557
1	8.807648	3.765634	0.397560
6	7.144794	4.533078	1.527763
1	7.563479	5.529958	1.621314
6	5.912063	4.233490	2.097403
1	5.366533	4.998469	2.641943

6	5.376870	2.956647	1.978288
1	4.418099	2.702047	2.413551

T_1 geometry optimized at PBE0(D3BJ)/6-311G(d,p)+SDD(Pd) with toluene as solvent

46	-0.215264	0.609604	-0.48143
7	0.001378	-2.354906	-1.738326
7	1.703670	-1.065144	-1.863057
7	1.184357	3.118763	-0.047568
7	-0.630479	3.408726	1.052899
7	-2.180127	0.099360	0.169576
7	4.203967	0.455985	1.464333
7	6.212413	-0.114733	0.346180
7	4.511199	-1.747334	0.610390
6	-4.779198	-1.995547	-3.127423
1	-4.765688	-0.922128	-2.917484
1	-5.794445	-2.357918	-2.942316
1	-4.563535	-2.133272	-4.192041
6	-3.762958	-2.723005	-2.260214
1	-3.807309	-3.802191	-2.454949
1	-4.021898	-2.588542	-1.203930
6	-2.345659	-2.220120	-2.492420
1	-2.311466	-1.135175	-2.349795
1	-2.038118	-2.414730	-3.527141
6	-1.349230	-2.860059	-1.540975
1	-1.633643	-2.674163	-0.505334
1	-1.310867	-3.942985	-1.682679
6	1.023322	-3.080431	-2.322757
1	0.893022	-4.105607	-2.626146
6	2.103506	-2.266366	-2.396143
1	3.101041	-2.446022	-2.758969
6	0.404838	-1.108126	-1.436824
6	2.386593	0.158616	-1.699553
6	1.579187	1.099120	-1.086542
6	2.104860	2.343860	-0.791133
6	3.400197	2.690375	-1.148092
1	3.824564	3.657485	-0.904487
6	4.177749	1.728665	-1.792185
1	5.201802	1.969077	-2.051747
6	3.693706	0.449908	-2.064579
1	4.337892	-0.289682	-2.526515
6	-0.022548	2.536103	0.229033
6	1.320123	4.326165	0.596543

1	2.207175	4.932739	0.524960
6	0.169467	4.514055	1.287206
1	-0.144688	5.326115	1.921498
6	-1.954260	3.214526	1.622983
1	-1.881818	3.345810	2.706986
1	-2.222049	2.175952	1.429609
6	-2.991108	4.154565	1.032475
1	-2.744541	5.190759	1.295510
1	-2.949760	4.084573	-0.059864
6	-4.395356	3.816194	1.511912
1	-4.655740	2.809742	1.163689
1	-4.410406	3.780425	2.608509
6	-5.429368	4.815077	1.017658
1	-6.435659	4.544414	1.348347
1	-5.438496	4.856791	-0.075413
1	-5.215535	5.822524	1.389001
6	-3.399601	1.618284	-1.389722
1	-2.497930	2.084127	-1.774156
6	-4.655780	1.961179	-1.863851
1	-4.725807	2.722458	-2.633148
6	-5.834459	1.341283	-1.401846
6	-5.731572	0.354648	-0.416295
1	-6.616800	-0.151413	-0.050646
6	-4.484394	-0.000075	0.077913
6	-3.315437	0.631543	-0.409020
6	-2.601771	-0.866180	1.045222
6	-4.016241	-1.012907	1.003976
6	-4.635718	-2.080169	1.619165
1	-5.711333	-2.200015	1.553525
6	-3.843277	-3.061776	2.274839
6	-2.468290	-2.902637	2.322674
1	-1.861708	-3.625571	2.853191
6	-1.793390	-1.783124	1.772767
6	-7.172559	1.725537	-2.028105
6	-8.343832	0.972246	-1.398535
1	-8.253019	-0.108972	-1.538508
1	-9.276893	1.289455	-1.872340
1	-8.428110	1.177407	-0.327113
6	-7.419763	3.229105	-1.850722
1	-7.472018	3.491597	-0.790970
1	-8.367129	3.510757	-2.321144
1	-6.628808	3.828796	-2.308173
6	-7.133618	1.388984	-3.526435
1	-6.341195	1.936618	-4.042807

1	-8.086885	1.652653	-3.995683
1	-6.959043	0.320280	-3.679884
6	-4.545493	-4.259882	2.902254
6	-3.570872	-5.227687	3.570965
1	-2.849571	-5.633949	2.855921
1	-4.127350	-6.067809	3.995735
1	-3.018426	-4.748848	4.384370
6	-5.302307	-5.021178	1.802797
1	-6.056073	-4.395635	1.318143
1	-5.811696	-5.889959	2.231582
1	-4.611254	-5.374670	1.031888
6	-5.540669	-3.765102	3.961635
1	-5.021281	-3.220612	4.755279
1	-6.061368	-4.615635	4.412837
1	-6.294040	-3.099258	3.533259
6	-0.371232	-1.608651	1.872409
6	0.535638	-2.671054	1.626665
1	0.145255	-3.673538	1.474912
6	1.874862	-2.431410	1.454453
1	2.546517	-3.233356	1.172670
6	2.411493	-1.121867	1.599710
6	1.532217	-0.096284	2.021252
1	1.940591	0.889458	2.205816
6	0.180269	-0.321091	2.104430
1	-0.482603	0.482074	2.409997
6	3.757365	-0.806072	1.237842
6	5.694940	-1.346823	0.187187
6	5.402867	0.739672	1.003249
6	6.513381	-2.326327	-0.565066
6	6.030518	-3.614812	-0.809232
1	5.054261	-3.879071	-0.420176
6	6.789041	-4.524058	-1.531413
1	6.405928	-5.523085	-1.713465
6	8.041153	-4.159383	-2.019970
1	8.634526	-4.871530	-2.584247
6	8.528213	-2.879293	-1.779559
1	9.504268	-2.590726	-2.156147
6	7.769931	-1.967496	-1.057010
1	8.131961	-0.965838	-0.859590
6	5.883365	2.127839	1.184094
6	7.112479	2.528115	0.658426
1	7.718766	1.789525	0.147913
6	7.535311	3.845633	0.784215
1	8.491807	4.147101	0.369443

6	6.738083	4.776990	1.440108
1	7.069902	5.805499	1.538976
6	5.513680	4.381235	1.974792
1	4.890836	5.101802	2.495856
6	5.089367	3.067435	1.847248
1	4.136801	2.741289	2.247771

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