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Coaxial Versus Perpendicular Structures for a Range of Binuclear Cyclopentadienylpalladium Derivatives

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Supporting Information

Tables S1 to S6 Total energies (E, in hartree) for the optimized $Cp_2Pd_2X_2$ (X = F, Cl, and CN) and $Cp_2Pd_2L_2$ (L = CO, CS, and $CNCH_3$)
Tables S7 to S10 Coordinates of $Cp_2Pd_2F_2$.
Tables S11 to S14 Coordinates of $Cp_2Pd_2Cl_2$.
Tables S15 to S20 Coordinates of $Cp_2Pd_2(CN)_2$.
Tables S21 to S24 Coordinates of $Cp_2Pd_2(CO)_2$.
Tables S25 to S28 Coordinates of $Cp_2Pd_2(CNCH_3)_2$.
Tables S29 to S32 Coordinates of $Cp_2Pd_2(CS)_2$.
Tables S33 to S36Harmonic vibrational frequencies of $Cp_2Pd_2F_2$.
Tables S37 to S40 Harmonic vibrational frequencies of $Cp_2Pd_2Cl_2$.
Tables S41 to S46 Harmonic vibrational frequencies of $Cp_2Pd_2(CN)_2$.
Tables S47 to S50 Harmonic vibrational frequencies of $Cp_2Pd_2(CO)_2$.
Tables S51 to S54 Harmonic vibrational frequencies of $Cp_2Pd_2(CNCH_3)_2$.
Tables S55 to S58 Harmonic vibrational frequencies of $Cp_2Pd_2(CS)_2$.
Complete Gaussian 09 reference (Reference 10)

Table S1 Total energies (E, in hartree) for the $Cp_2Pd_2F_2$ structures. None of the four structures has any imaginary vibrational frequencies.

		2F-1S (C_1)	**2F-2S** (C_{2v})	**2F-3S** (C_{2v})	**2F-4S** (C_1)
MPW1PW91	E	-842.445289	-842.425057	-842.422985	-842.418790
BP86	E	-842.719341	-842.715616	-842.691221	-842.694784

Table S2 Total energies (E, in hartree) for the $Cp_2Pd_2Cl_2$ structures. None of the four structures has any imaginary vibrational frequencies.

		2Cl-1S (C_{2v})	**2Cl-2S**(C_{2v})	**2Cl-3S**(C_1)	**2Cl-4S**(C_1)
MPW1PW91	E	-1563.206756	-1563.204405	-1563.194101	-1563.193070
BP86	E	-1563.489969	-1563.467372	-1563.465796	-1563.465076

Table S3 Total energies (E, in hartree) for the $Cp_2Pd_2(CN)_2$ structures. None of these structures has any imaginary vibrational frequencies.

	2CN-1S (C_1)	**2CN-2S** (C_2/C_1)	**2CN-3S** (C_s)	**2CN-4S** (C_1)	**2CN-5S** (C_{2v})	**2CN-6S** (C_{2h})
MPW1PW91	-828.396983	-828.388773	-828.388071	-828.376571	-828.373895	-828.364871
BP86	-828.676915	-828.667757	-828.665735	-828.658730	-828.655692	-828.658882

Table S4 Total energies (E, in hartree) and numbers of imaginary vibrational frequencies (Nimag) for the $Cp_2Pd_2(CO)_2$ structures.

		2CO-1S (C_{2v})	**2CO-2S** (C_{2h})	**2CO-3S** (C_{2v})	**2CO-4S** (C_1)
MPW1PW91	E	-869.416094	-869.412878	-869.411456	-869.404737
	Nimag	0	0	0	0
BP86	E	-869.723284	-869.712856	-869.710819	-869.708258
	Nimag	1(11i)[a]	0	0	0

[a] Denotes the imaginary vibrational frequency diminishing after using the finer (120, 974) grid.

Table S5 Total energies (E, in hartree) for the $Cp_2Pd_2(CNCH_3)_2$ structures. None of these structures has any imaginary vibrational frequencies.

		2CNCH$_3$-1S (C_s)	**2CNCH$_3$-2S** (C_2)	**2CNCH$_3$-3S** (C_2)	**2CNCH$_3$-4S** (C_1)
MPW1PW91	E	-908.139419	-908.138843	-908.138598	-908.138504
BP86	E	-908.438575	-908.446189	-908.437272	-908.446007

Table S6 Total energies (E, in hartree) and numbers of imaginary vibrational frequencies (Nimag) for the $Cp_2Pd_2(CS)_2$ structures.

		2CS-1S (C_{2v})	2CS-2S (C_1)	2CS-3S (C_{2h})	2CS-4S (C_{2v})
MPW1PW91	E	-1515.300659	-1515.270062	-1515.264746	-1515.264217
	Nimg	2(<4i)[a]	0	0	0
BP86	E	-1515.618811	-1515.589108	-1515.583574	-1515.582663
	Nimg	0	0	0	0

[a] These imaginary vibrational frequencies are eliminated using the finer (120, 974) grid.

Table S7 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2F_2$ **2F-1S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	-0.037596	-1.422679	-0.170338	-0.083536	-1.426768	-0.167837
Pd	-0.167324	1.061630	-0.099026	-0.130471	1.086259	-0.098431
C	-2.421868	-0.831475	-0.709869	-2.444159	-0.823268	-0.707282
C	-2.457356	0.566357	-0.516288	-2.447483	0.596346	-0.553252
C	-2.123834	0.839792	0.860286	-2.121683	0.904043	0.830948
C	-2.087499	-1.451956	0.549134	-2.136329	-1.420301	0.585941
C	-1.885277	-0.413548	1.506612	-1.923091	-0.349252	1.524821
C	1.646209	-0.763748	-1.375581	1.618868	-0.828566	-1.391916
C	1.579235	0.719470	-1.339398	1.597245	0.667537	-1.363387
C	1.967866	1.155656	-0.063640	2.017565	1.104165	-0.074760
C	2.085733	-1.228845	-0.121465	2.057549	-1.305221	-0.118801
C	2.518141	-0.029684	0.705303	2.540114	-0.104578	0.701716
F	2.117110	-0.081595	2.025263	2.132201	-0.136353	2.046881
H	2.209116	2.183013	0.190353	2.318701	2.130381	0.163853
H	1.469294	1.344931	-2.219440	1.517603	1.293975	-2.258714
H	3.619720	0.027312	0.720794	3.654312	-0.085091	0.727165
H	1.638885	-1.331329	-2.302165	1.599565	-1.404623	-2.325485
H	2.527019	-2.207953	0.050594	2.483565	-2.302642	0.052993
H	-2.704524	-1.351116	-1.618707	-2.742460	-1.366114	-1.609596
H	-2.218699	-2.505659	0.789930	-2.297075	-2.472410	0.859249
H	-1.668785	-0.551184	2.559109	-1.706510	-0.461907	2.590395
H	-2.766702	1.305125	-1.246761	-2.743654	1.324733	-1.313765
H	-2.229143	1.800494	1.353833	-2.224692	1.886948	1.303745
F	-0.270215	3.028543	-0.120526	-0.195157	3.077986	-0.107513

Table S8 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2F_2$ **2F-2S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	0.000000	1.236073	-0.035303	0.000000	1.261743	-0.043756
Pd	0.000000	-1.236073	-0.035303	0.000000	-1.261743	-0.043756
C	-1.846269	0.735668	1.017426	2.215606	1.176912	-0.268439
C	-1.846269	-0.735668	1.017426	2.404958	0.000000	-1.074678
C	-2.164665	-1.168833	-0.307395	2.215606	-1.176912	-0.268439
C	-2.164665	1.168833	-0.307395	1.817017	0.744381	1.051868
C	-2.282150	0.000000	-1.119908	1.817017	-0.744381	1.051868
C	1.846269	0.735668	1.017426	-2.215606	1.176912	-0.268439
C	1.846269	-0.735668	1.017426	-2.404958	0.000000	-1.074678
C	2.164665	-1.168833	-0.307395	-2.215606	-1.176912	-0.268439
C	2.164665	1.168833	-0.307395	-1.817017	0.744381	1.051868
C	2.282150	0.000000	-1.119908	-1.817017	-0.744381	1.051868
F	0.000000	3.258025	-0.065667	0.000000	3.293160	-0.177534
H	2.374187	-2.190023	-0.607363	-2.445130	-2.207539	-0.557410
H	1.894577	-1.350104	1.910077	-2.645600	0.000000	-2.142995
H	2.454295	0.000000	-2.191400	-1.845172	-1.359556	1.957671
H	1.894577	1.350104	1.910077	-2.445130	2.207539	-0.557410
H	2.374187	2.190023	-0.607363	-1.845172	1.359556	1.957671
H	-1.894577	1.350104	1.910077	2.445130	2.207539	-0.557410
H	-2.374187	2.190023	-0.607363	1.845172	1.359556	1.957671
H	-2.454295	0.000000	-2.191400	1.845172	-1.359556	1.957671
H	-1.894577	-1.350104	1.910077	2.645600	0.000000	-2.142995
H	-2.374187	-2.190023	-0.607363	2.445130	-2.207539	-0.557410
F	0.000000	-3.258025	-0.065667	0.000000	-3.293160	-0.177534

Table S9 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2F_2$ **2F-3S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	-0.682324	3.762241	1.110200	-0.687506	3.927318	1.050736
H	-1.337475	3.874814	1.965971	-1.350364	4.132978	1.896082
C	0.682324	3.762241	1.110200	0.687506	3.927318	1.050736
H	1.337475	3.874814	1.965971	1.350364	4.132978	1.896082
C	1.128178	3.426156	-0.261651	1.139585	3.446821	-0.293499
H	2.164737	3.388126	-0.580085	2.186309	3.388662	-0.611403
C	0.000000	3.486284	-1.129679	0.000000	3.425373	-1.177958
H	0.000000	3.415440	-2.210305	0.000000	3.295205	-2.263544
C	-1.128178	3.426156	-0.261651	-1.139585	3.446821	-0.293499
H	-2.164737	3.388126	-0.580085	-2.186309	3.388662	-0.611403
C	0.000000	-3.486284	-1.129679	0.000000	-3.425373	-1.177958
H	0.000000	-3.415440	-2.210305	0.000000	-3.295205	-2.263544
C	-1.128178	-3.426156	-0.261651	-1.139585	-3.446821	-0.293499
H	-2.164737	-3.388126	-0.580085	-2.186309	-3.388662	-0.611403
C	-0.682324	-3.762241	1.110200	-0.687506	-3.927318	1.050736
H	-1.337475	-3.874814	1.965971	-1.350364	-4.132978	1.896082
C	0.682324	-3.762241	1.110200	0.687506	-3.927318	1.050736
H	1.337475	-3.874814	1.965971	1.350364	-4.132978	1.896082
C	1.128178	-3.426156	-0.261651	1.139585	-3.446821	-0.293499
H	2.164737	-3.388126	-0.580085	2.186309	-3.388662	-0.611403
F	1.330915	0.000000	0.099666	1.325176	0.000000	0.227035
F	-1.330915	0.000000	0.099666	-1.325176	0.000000	0.227035
Pd	0.000000	1.579661	-0.105717	0.000000	1.590346	-0.094961
Pd	0.000000	-1.579661	-0.105717	0.000000	-1.590346	-0.094961

Table S10 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2F_2$ **2F-4S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	-1.141278	0.109160	-0.092188	-1.160200	0.117306	-0.081640
Pd	1.997890	-0.708242	-0.179344	2.024278	-0.702975	-0.177906
C	-3.451986	0.310730	-0.332702	-3.484137	0.338041	-0.333811
C	-2.972006	0.206118	1.031237	-3.020186	0.212752	1.046908
C	-2.590372	-1.176278	1.277477	-2.631687	-1.183617	1.276360
C	-3.112191	-0.885275	-0.962706	-3.166347	-0.874846	-0.979621
C	-2.593813	-1.816441	0.045584	-2.655203	-1.825352	0.026756
C	0.239084	1.197341	1.169242	0.207739	1.211230	1.167322
C	1.663291	1.054489	0.753793	1.659223	1.039151	0.810905
C	1.832723	2.015829	-0.348013	1.895899	1.962742	-0.320908
C	-0.361570	2.153964	0.305399	-0.346118	2.168925	0.232762
C	0.640266	2.613330	-0.642105	0.707285	2.576793	-0.689369
F	0.375064	-0.447724	-1.382801	0.368290	-0.485043	-1.383089
H	2.774884	2.182518	-0.859715	2.875692	2.121246	-0.783242
H	2.414141	0.996702	1.545456	2.390431	0.953440	1.632474
H	0.451162	3.315525	-1.446588	0.565566	3.257223	-1.535044
H	-0.084765	0.982534	2.183201	-0.139872	1.072973	2.198187
H	-1.280988	2.694087	0.514260	-1.258675	2.754126	0.400055
H	-3.869700	1.195166	-0.797018	-3.896488	1.238566	-0.795450
H	-3.236222	-1.115304	-2.014752	-3.296403	-1.095186	-2.043258
H	-2.266270	-2.829874	-0.155553	-2.332545	-2.849131	-0.183395
H	-3.108523	0.959226	1.800775	-3.158258	0.965010	1.831174
H	-2.249161	-1.582874	2.221310	-2.290730	-1.606474	2.224573
F	3.546128	-1.028140	0.906783	3.608920	-1.028946	0.890778

Table S11 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2Cl_2$ **2Cl-1S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	0.000000	1.246665	-0.034157	0.000000	1.271595	-0.029346
Pd	0.000000	-1.246665	-0.034157	0.000000	-1.271595	-0.029346
C	-1.865092	0.734238	1.008018	-1.840509	0.742793	1.054577
C	-1.865092	-0.734238	1.008018	-1.840509	-0.742793	1.054577
C	-2.166580	-1.169006	-0.320331	-2.213836	-1.177503	-0.272007
C	-2.166580	1.169006	-0.320331	-2.213836	1.177503	-0.272007
C	-2.265057	0.000000	-1.136182	-2.377294	0.000000	-1.084499
C	1.865092	0.734238	1.008018	1.840509	0.742793	1.054577
C	1.865092	-0.734238	1.008018	1.840509	-0.742793	1.054577
C	2.166580	-1.169006	-0.320331	2.213836	-1.177503	-0.272007
C	2.166580	1.169006	-0.320331	2.213836	1.177503	-0.272007
C	2.265057	0.000000	-1.136182	2.377294	0.000000	-1.084499
H	2.402435	-2.184000	-0.619818	2.466020	-2.202368	-0.560592
H	1.917929	-1.349314	1.899795	1.874153	-1.359162	1.959008
H	2.425506	0.000000	-2.209459	2.598668	0.000000	-2.156944
H	1.917929	1.349314	1.899795	1.874153	1.359162	1.959008
H	2.402435	2.184000	-0.619818	2.466020	2.202368	-0.560592
H	-1.917929	1.349314	1.899795	-1.874153	1.359162	1.959008
H	-2.402435	2.184000	-0.619818	-2.466020	2.202368	-0.560592
H	-2.425506	0.000000	-2.209459	-2.598668	0.000000	-2.156944
H	-1.917929	-1.349314	1.899795	-1.874153	-1.359162	1.959008
H	-2.402435	-2.184000	-0.619818	-2.466020	-2.202368	-0.560592
Cl	0.000000	-3.630152	-0.012613	0.000000	-3.667407	-0.127871
Cl	0.000000	3.630152	-0.012613	0.000000	3.667407	-0.127871

Table S12 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2Cl_2$ **2Cl-2S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	0.000000	3.526764	1.308574	0.000000	3.300713	1.465275
H	0.000000	3.366565	2.379129	0.000000	2.977756	2.509259
C	1.129275	3.536664	0.444463	1.141361	3.469790	0.605476
H	2.165410	3.471713	0.758924	2.187417	3.362056	0.911008
C	0.684730	3.924331	-0.909977	0.689787	4.112567	-0.664376
H	1.339551	4.075112	-1.759760	1.351383	4.425410	-1.476907
C	-0.684730	3.924331	-0.909977	-0.689787	4.112567	-0.664376
H	-1.339551	4.075112	-1.759760	-1.351383	4.425410	-1.476907
C	-1.129275	3.536664	0.444463	-1.141361	3.469790	0.605476
H	-2.165410	3.471713	0.758924	-2.187417	3.362056	0.911008
C	-0.684730	-3.924331	-0.909977	-0.689787	-4.112567	-0.664376
H	-1.339551	-4.075112	-1.759760	-1.351383	-4.425410	-1.476907
C	-1.129275	-3.536664	0.444463	-1.141361	-3.469790	0.605476
H	-2.165410	-3.471713	0.758924	-2.187417	-3.362056	0.911008
C	0.000000	-3.526764	1.308574	0.000000	-3.300713	1.465275
H	0.000000	-3.366565	2.379129	0.000000	-2.977756	2.509259
C	1.129275	-3.536664	0.444463	1.141361	-3.469790	0.605476
H	2.165410	-3.471713	0.758924	2.187417	-3.362056	0.911008
C	0.684730	-3.924331	-0.909977	0.689787	-4.112567	-0.664376
H	1.339551	-4.075112	-1.759760	1.351383	-4.425410	-1.476907
Pd	0.000000	1.695517	0.049605	0.000000	1.667431	0.009355
Pd	0.000000	-1.695517	0.049605	0.000000	-1.667431	0.009355
Cl	-1.666177	0.000000	-0.289680	-1.646471	0.000000	-0.581921
Cl	1.666177	0.000000	-0.289680	1.646471	0.000000	-0.581921

Table S13 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2Cl_2$ **2Cl-3S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	-1.002096	1.214596	-0.292838	-1.032902	1.200858	-0.287053
Pd	0.851083	-0.458743	-0.122732	0.875030	-0.449211	-0.124249
C	1.188902	2.529926	-0.373541	1.065822	2.611250	-0.360972
C	2.152267	1.544471	-0.089775	2.082174	1.645469	-0.112797
C	1.850492	0.975524	1.204841	1.833315	1.046922	1.192409
C	0.282751	2.612735	0.748445	0.181586	2.652212	0.798277
C	0.686937	1.638061	1.708523	0.649904	1.672927	1.743505
C	-1.501129	-0.270846	-1.786172	-1.491908	-0.279168	-1.804938
C	-0.412424	-1.272143	-1.701765	-0.368903	-1.260739	-1.734311
C	-0.579617	-2.022123	-0.526617	-0.522735	-2.047770	-0.556178
C	-2.337162	-0.413697	-0.660750	-2.335568	-0.465308	-0.664322
C	-1.922681	-1.670739	0.076901	-1.890577	-1.742220	0.046152
H	-0.077260	-2.958846	-0.310268	-0.004843	-2.993570	-0.365774
H	0.252890	-1.520492	-2.522322	0.298250	-1.488623	-2.572833
H	-2.635264	-2.476731	-0.146898	-2.592366	-2.568721	-0.189918
H	-1.745644	0.259904	-2.702492	-1.760512	0.251079	-2.727368
H	-3.360037	-0.051057	-0.596418	-3.381548	-0.138415	-0.603132
H	1.179513	3.174611	-1.245325	1.017282	3.278335	-1.227161
H	-0.401857	3.436203	0.946026	-0.534679	3.453912	1.026023
H	0.250112	1.488319	2.688301	0.233469	1.485089	2.736460
H	3.018516	1.301310	-0.694007	2.953117	1.449189	-0.744460
H	2.514361	0.340291	1.781354	2.547377	0.436976	1.755605
Cl	-1.939329	-1.533176	1.860536	-1.922310	-1.648910	1.863089
Cl	2.615874	-1.976809	-0.077141	2.702775	-1.924177	-0.065942

Table S14 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2Cl_2$ **2Cl-4S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	1.357804	0.106505	0.006480	1.324477	0.122295	-0.011306
Pd	-1.892435	-0.471990	0.336428	-1.841936	-0.449884	0.355092
C	3.688579	0.068980	-0.088505	3.669960	0.022908	-0.082693
C	3.036645	-0.203032	-1.351834	3.032619	-0.299667	-1.356142
C	2.462282	-1.535617	-1.300090	2.410237	-1.619308	-1.244266
C	3.296949	-0.948649	0.783272	3.257357	-0.966482	0.836898
C	2.547966	-1.956256	0.021973	2.486683	-1.994987	0.108940
C	-0.089852	1.088137	-1.287669	-0.110203	1.062251	-1.352977
C	-1.467330	1.192119	-0.726242	-1.500274	1.200530	-0.807012
C	-1.406973	2.335759	0.210708	-1.449797	2.382153	0.094126
C	0.692343	2.110605	-0.694301	0.688221	2.113522	-0.769540
C	-0.149205	2.850185	0.242827	-0.171599	2.895489	0.127413
H	-2.254530	2.676831	0.795436	-2.312375	2.755037	0.655534
H	-2.267480	1.194602	-1.472043	-2.323792	1.127292	-1.538738
H	0.197984	3.668547	0.864226	0.171954	3.740125	0.733481
H	0.092841	0.644571	-2.261466	0.071413	0.600727	-2.330175
H	1.616025	2.507373	-1.107072	1.616109	2.507537	-1.202517
H	4.262552	0.953081	0.158330	4.267271	0.911785	0.133749
H	3.529423	-1.016570	1.839753	3.484333	-0.992714	1.906575
H	2.133196	-2.866668	0.438363	2.043435	-2.885857	0.562484
H	3.141015	0.395370	-2.251293	3.165201	0.258282	-2.289418
H	1.955831	-2.042274	-2.111988	1.890043	-2.153364	-2.043132
Cl	-3.620635	-1.014441	-1.034340	-3.538328	-1.179707	-0.994503
Cl	-0.113617	-0.121790	1.885702	-0.117537	0.028047	1.951532

Table S15 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CN)_2$ **2CN-1S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	-1.362290	0.710164	-0.347421	-1.386273	0.675361	-0.341473
Pd	0.997533	-0.170754	-0.190669	1.022199	-0.137675	-0.191284
C	-0.503532	2.611965	0.254782	-0.653421	2.626994	0.319632
C	0.704795	2.555275	-0.499118	0.568738	2.665828	-0.441024
C	1.686939	1.867403	0.268037	1.589489	1.973746	0.292729
C	-0.277183	1.913819	1.502364	-0.400039	1.855672	1.531839
C	1.061975	1.465847	1.515421	0.980763	1.462302	1.521970
C	-1.366872	-1.012718	-1.659728	-1.336986	-1.029311	-1.693470
C	0.004758	-1.554432	-1.578063	0.061304	-1.527942	-1.631720
C	0.180652	-2.181011	-0.334243	0.271418	-2.182132	-0.384219
C	-2.046807	-1.309004	-0.462431	-2.005890	-1.373697	-0.478039
C	-1.172028	-2.247258	0.366211	-1.089763	-2.323725	0.320591
H	0.976677	-2.877585	-0.096227	1.093217	-2.873414	-0.173211
H	0.672334	-1.648816	-2.428830	0.729639	-1.586432	-2.498025
H	-1.556476	-3.275650	0.250621	-1.444257	-3.369580	0.157939
H	-1.826311	-0.711554	-2.597126	-1.820305	-0.730207	-2.631740
H	-3.127827	-1.329716	-0.350921	-3.095118	-1.446253	-0.365711
H	-1.327020	3.293731	0.050277	-1.515594	3.285675	0.148899
H	-0.965380	1.846830	2.337703	-1.080241	1.730714	2.379730
H	1.566016	1.002716	2.355947	1.515220	1.006544	2.360754
H	0.872738	3.026389	-1.460355	0.710669	3.186027	-1.392428
H	2.752878	1.866119	0.071001	2.663660	2.028687	0.092561
C	-1.158253	-1.962836	1.803304	-1.085000	-2.101488	1.777057
N	-1.175847	-1.754796	2.946920	-1.109688	-1.941281	2.945357
C	2.825296	-0.879712	-0.096606	2.885260	-0.760706	-0.093632
N	3.904811	-1.332259	-0.069710	4.006156	-1.155656	-0.062817

Table S16 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CN)_2$ **2CN-2S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	1.332448	-3.724373	-0.084361	1.358800	-3.820703	-0.028102
H	2.399966	-3.595175	-0.224145	2.443067	-3.702827	-0.120652
C	0.674980	-3.918314	1.206644	0.633526	-3.999658	1.239002
H	1.150018	-3.830001	2.175598	1.066057	-3.915432	2.238719
C	-0.674980	-4.092740	0.948016	-0.720952	-4.158177	0.911637
H	-1.469180	-4.174413	1.680701	-1.556979	-4.228745	1.613248
C	-0.867509	-4.103907	-0.503587	-0.846324	-4.184376	-0.559407
H	-1.823311	-4.226797	-1.000172	-1.787510	-4.298243	-1.105409
C	0.383633	-4.017868	-1.128658	0.443293	-4.094317	-1.129491
H	0.583231	-4.022331	-2.192425	0.696089	-4.097675	-2.192062
C	0.867509	4.103907	-0.503587	0.846323	4.184376	-0.559407
H	1.823311	4.226797	-1.000172	1.787510	4.298244	-1.105408
C	0.674980	4.092740	0.948016	0.720952	4.158177	0.911637
H	1.469180	4.174413	1.680701	1.556979	4.228745	1.613248
C	-0.674980	3.918314	1.206644	-0.633526	3.999658	1.239002
H	-1.150018	3.830001	2.175598	-1.066057	3.915432	2.238719
C	-1.332448	3.724373	-0.084361	-1.358800	3.820702	-0.028102
H	-2.399966	3.595175	-0.224145	-2.443067	3.702826	-0.120652
C	-0.383633	4.017868	-1.128658	-0.443293	4.094317	-1.129491
H	-0.583231	4.022331	-2.192425	-0.696089	4.097675	-2.192062
C	1.211117	-0.450102	-0.054133	1.207748	-0.484566	-0.051289
N	1.644688	0.649204	-0.061489	1.548317	0.667246	-0.066977
Pd	-0.034917	1.993954	-0.050275	-0.078264	2.043843	-0.037504
Pd	0.034917	-1.993954	-0.050275	0.078264	-2.043843	-0.037504
N	-1.644688	-0.649204	-0.061489	-1.548317	-0.667245	-0.066977
C	-1.211117	0.450102	-0.054133	-1.207748	0.484566	-0.051289

Table S17 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CN)_2$ **2CN-3S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	-0.276069	4.039208	1.136666	-0.266224	4.098216	1.147741
H	-0.600226	4.048037	2.171067	-0.593769	4.105723	2.191690
C	1.113554	4.074860	0.694858	1.136135	4.120361	0.702026
H	1.979666	4.044570	1.344559	2.009807	4.082862	1.357795
C	1.113554	4.074860	-0.694858	1.136135	4.120361	-0.702026
H	1.979666	4.044570	-1.344559	2.009807	4.082862	-1.357795
C	-0.276069	4.039208	-1.136666	-0.266224	4.098216	-1.147741
H	-0.600226	4.048037	-2.171067	-0.593769	4.105723	-2.191690
C	-1.118652	4.161579	0.000000	-1.117224	4.218652	0.000000
H	-2.200235	4.202284	0.000000	-2.208489	4.263046	0.000000
C	-0.241591	-3.967390	1.129624	-0.215657	-4.019590	1.142427
H	-0.561760	-3.950076	2.165687	-0.539327	-4.008724	2.188199
C	1.159712	-4.089102	0.686790	1.196118	-4.165912	0.692795
H	2.022583	-4.078077	1.341611	2.067229	-4.167669	1.353518
C	1.159712	-4.089102	-0.686790	1.196118	-4.165912	-0.692795
H	2.022583	-4.078077	-1.341611	2.067229	-4.167669	-1.353518
C	-0.241591	-3.967390	-1.129624	-0.215657	-4.019590	-1.142427
H	-0.561760	-3.950076	-2.165687	-0.539327	-4.008724	-2.188199
C	-1.092231	-4.111423	0.000000	-1.078671	-4.144055	0.000000
H	-2.174174	-4.140604	0.000000	-2.170676	-4.173418	0.000000
C	-0.064391	0.549865	1.202048	-0.075206	0.571906	1.190360
N	-0.074149	-0.589386	1.493337	-0.091455	-0.595166	1.442411
Pd	-0.112145	-2.087941	0.000000	-0.138403	-2.117718	0.000000
Pd	-0.046492	2.098172	0.000000	-0.043226	2.128826	0.000000
N	-0.074149	-0.589386	-1.493337	-0.091455	-0.595166	-1.442411
C	-0.064391	0.549865	-1.202048	-0.075206	0.571906	-1.190360

Table S18 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CN)_2$ **2CN-4S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	3.577631	-0.735637	0.026699	3.649053	-0.486897	0.008754
H	3.939073	-1.635478	-0.458712	4.171323	-1.191614	-0.645539
C	3.569421	0.562115	-0.529579	3.422872	0.890299	-0.254021
H	3.860609	0.844410	-1.532899	3.690841	1.443991	-1.156258
C	2.876437	1.375765	0.418274	2.586428	1.367535	0.830320
H	2.630798	2.423452	0.285907	2.189097	2.383504	0.916853
C	2.779658	0.639946	1.693199	2.556917	0.342878	1.895474
H	2.362377	1.035300	2.611068	2.048911	0.443745	2.857662
C	3.179389	-0.649061	1.447696	3.160052	-0.800681	1.377338
H	3.148591	-1.487579	2.133082	3.231623	-1.781751	1.855023
C	-2.971304	-0.073927	1.646373	-2.758225	0.465993	1.753654
H	-2.650498	-0.245546	2.665605	-2.347770	0.787864	2.714258
C	-3.276872	-1.072437	0.673632	-3.073357	-0.849428	1.372007
H	-3.322187	-2.140709	0.853915	-2.978691	-1.752447	1.980753
C	-3.739837	-0.407996	-0.549439	-3.533269	-0.812273	-0.031478
H	-4.092405	-0.910608	-1.441503	-3.879450	-1.678467	-0.603426
C	-3.548473	0.952416	-0.375650	-3.580182	0.554585	-0.459156
H	-3.703611	1.730409	-1.113046	-3.887341	0.920241	-1.441251
C	-2.990190	1.160261	0.958551	-2.977604	1.327697	0.588899
H	-2.731643	2.127392	1.374419	-2.790727	2.404952	0.553930
Pd	1.441937	-0.112942	-0.255329	1.385044	-0.126143	-0.249016
Pd	-1.421233	-0.146824	-0.074768	-1.378147	-0.156591	-0.171667
C	-0.209483	-1.579688	-0.606465	-0.192484	-1.563186	-0.812769
N	0.714481	-2.242798	-0.945137	0.742220	-2.198934	-1.238622
C	-0.040607	1.317125	-0.740012	-0.024685	1.249684	-0.999205
N	-0.089925	2.424921	-1.136729	-0.053391	2.328720	-1.518450

Table S19 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CN)_2$ **2CN-5S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	0.000000	3.446730	-1.020380	0.000000	3.494120	-0.931138
H	0.000000	3.530772	-2.099216	0.000000	3.626253	-2.015086
C	-1.130790	3.268964	-0.180745	-1.142955	3.293091	-0.088465
H	-2.167006	3.265724	-0.500278	-2.188668	3.308995	-0.411185
C	-0.688062	3.283271	1.224745	-0.695012	3.246765	1.327635
H	-1.344770	3.219767	2.083690	-1.357596	3.147843	2.191308
C	0.688062	3.283271	1.224745	0.695012	3.246765	1.327635
H	1.344770	3.219767	2.083690	1.357596	3.147843	2.191308
C	1.130790	3.268964	-0.180745	1.142955	3.293091	-0.088465
H	2.167006	3.265724	-0.500278	2.188668	3.308995	-0.411185
C	1.130790	-3.268964	-0.180745	1.142955	-3.293091	-0.088465
H	2.167006	-3.265724	-0.500278	2.188668	-3.308995	-0.411185
C	0.000000	-3.446730	-1.020380	0.000000	-3.494120	-0.931138
H	0.000000	-3.530772	-2.099216	0.000000	-3.626253	-2.015086
C	-1.130790	-3.268964	-0.180745	-1.142955	-3.293091	-0.088465
H	-2.167006	-3.265724	-0.500278	-2.188668	-3.308995	-0.411185
C	-0.688062	-3.283271	1.224745	-0.695012	-3.246765	1.327635
H	-1.344770	-3.219767	2.083690	-1.357596	-3.147843	2.191308
C	0.688062	-3.283271	1.224745	0.695012	-3.246765	1.327635
H	1.344770	-3.219767	2.083690	1.357596	-3.147843	2.191308
Pd	0.000000	1.359434	-0.100501	0.000000	1.352363	-0.123934
Pd	0.000000	-1.359434	-0.100501	0.000000	-1.352363	-0.123934
C	1.590915	0.000000	-0.195972	1.571258	0.000000	-0.332737
N	2.769185	0.000000	-0.239206	2.766507	0.000000	-0.447286
C	-1.590915	0.000000	-0.195972	-1.571258	0.000000	-0.332737
N	-2.769185	0.000000	-0.239206	-2.766507	0.000000	-0.447286

Table S20 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CN)_2$ **2CN-6S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	-0.016624	1.258825	0.000000	-0.015074	1.285314	0.000000
Pd	0.016624	-1.258825	0.000000	0.015074	-1.285314	0.000000
C	-2.153936	1.362491	0.000000	-2.169199	1.405800	0.000000
C	-2.007998	0.516360	1.142158	-2.029639	0.550485	1.153997
C	-2.007998	-0.872226	0.713472	-2.029639	-0.850204	0.720518
C	-2.007998	0.516360	-1.142158	-2.029639	0.550485	-1.153997
C	-2.007998	-0.872226	-0.713472	-2.029639	-0.850204	-0.720518
C	2.007998	0.872226	0.713472	2.029639	0.850204	0.720518
C	2.007998	-0.516360	1.142158	2.029639	-0.550485	1.153997
C	2.153936	-1.362491	0.000000	2.169199	-1.405800	0.000000
C	2.007998	0.872226	-0.713472	2.029639	0.850204	-0.720518
C	2.007998	-0.516360	-1.142158	2.029639	-0.550485	-1.153997
H	2.405180	-2.415780	0.000000	2.426941	-2.467994	0.000000
H	2.051996	-0.846574	2.174438	2.074202	-0.883711	2.195756
H	2.051996	-0.846574	-2.174438	2.074202	-0.883711	-2.195756
H	2.255247	1.713702	1.350672	2.289973	1.697426	1.362083
H	2.255247	1.713702	-1.350672	2.289973	1.697426	-1.362083
H	-2.405180	2.415780	0.000000	-2.426941	2.467994	0.000000
H	-2.051996	0.846574	-2.174438	-2.074202	0.883711	-2.195756
H	-2.255247	-1.713702	-1.350672	-2.289973	-1.697426	-1.362083
H	-2.051996	0.846574	2.174438	-2.074202	0.883711	2.195756
H	-2.255247	-1.713702	1.350672	-2.289973	-1.697426	1.362083
C	-0.119783	-3.300381	0.000000	-0.154117	-3.324622	0.000000
N	-0.209001	-4.468326	0.000000	-0.267220	-4.507572	0.000000
C	0.119783	3.300381	0.000000	0.154117	3.324622	0.000000
N	0.209001	4.468326	0.000000	0.267220	4.507572	0.000000

Table S21 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CO)_2$ **2CO-1S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	0.000000	3.519354	-0.808406	0.715824	3.488982	-0.495932
H	0.000000	3.742152	-1.868014	1.365204	3.699974	-1.349719
C	-1.145539	3.323734	0.017836	-0.715824	3.488982	-0.495932
H	-2.178346	3.391727	-0.304412	-1.365204	3.699974	-1.349719
C	-0.702264	3.133165	1.377090	-1.155245	3.188244	0.858572
H	-1.347140	2.987438	2.235464	-2.197680	3.118455	1.183025
C	0.702264	3.133165	1.377090	0.000000	3.060031	1.694816
H	1.347140	2.987438	2.235464	0.000000	2.829669	2.763346
C	1.145539	3.323734	0.017836	1.155245	3.188244	0.858572
H	2.178346	3.391727	-0.304412	2.197680	3.118455	1.183025
C	0.702264	-3.133165	1.377090	0.000000	-3.060031	1.694816
H	1.347140	-2.987438	2.235464	0.000000	-2.829669	2.763346
C	1.145539	-3.323734	0.017836	1.155245	-3.188244	0.858572
H	2.178346	-3.391727	-0.304412	2.197680	-3.118455	1.183025
C	0.000000	-3.519354	-0.808406	0.715824	-3.488982	-0.495932
H	0.000000	-3.742152	-1.868014	1.365204	-3.699974	-1.349719
C	-1.145539	-3.323734	0.017836	-0.715824	-3.488982	-0.495932
H	-2.178346	-3.391727	-0.304412	-1.365204	-3.699974	-1.349719
C	-0.702264	-3.133165	1.377090	-1.155245	-3.188244	0.858572
H	-1.347140	-2.987438	2.235464	-2.197680	-3.118455	1.183025
Pd	0.000000	1.332066	-0.096573	0.000000	1.333191	-0.105135
Pd	0.000000	-1.332066	-0.096573	0.000000	-1.333191	-0.105135
C	1.433153	0.000000	-0.500216	1.406502	0.000000	-0.638347
O	2.561729	0.000000	-0.804889	2.528630	0.000000	-1.035527
C	-1.433153	0.000000	-0.500216	-1.406502	0.000000	-0.638347
O	-2.561729	0.000000	-0.804889	-2.528630	0.000000	-1.035527

Table S22 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CO)_2$ **2CO-2S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
Pd	0.000000	0.000000	1.349508	0.000000	0.000000	1.372504
Pd	0.000000	0.000000	-1.349508	0.000000	0.000000	-1.372504
C	0.000000	2.174272	1.162291	0.000000	2.196095	1.172617
C	-0.818189	1.991653	0.000000	-0.825491	1.990857	0.000000
C	0.000000	2.174272	-1.162291	0.000000	2.196095	-1.172617
C	1.345148	2.476152	0.686892	1.348835	2.525995	0.694460
C	1.345148	2.476152	-0.686892	1.348835	2.525995	-0.694460
C	-1.345148	-2.476152	0.686892	-1.348835	-2.525995	0.694460
C	-1.345148	-2.476152	-0.686892	-1.348835	-2.525995	-0.694460
C	0.000000	-2.174272	-1.162291	0.000000	-2.196095	-1.172617
C	0.000000	-2.174272	1.162291	0.000000	-2.196095	1.172617
C	0.818189	-1.991653	0.000000	0.825491	-1.990857	0.000000
H	0.392305	-2.527941	-2.110661	0.402613	-2.547647	-2.129029
H	-2.203645	-2.647587	-1.327701	-2.210464	-2.716279	-1.342650
H	1.902906	-1.978691	0.000000	1.919938	-1.966678	0.000000
H	-2.203645	-2.647587	1.327701	-2.210464	-2.716279	1.342650
H	0.392305	-2.527941	2.110661	0.402613	-2.547647	2.129029
H	-0.392305	2.527941	2.110661	-0.402613	2.547647	2.129029
H	2.203645	2.647587	1.327701	2.210464	2.716279	1.342650
H	2.203645	2.647587	-1.327701	2.210464	2.716279	-1.342650
H	-1.902906	1.978691	0.000000	-1.919938	1.966678	0.000000
H	-0.392305	2.527941	-2.110661	-0.402613	2.547647	-2.129029
C	0.000000	0.000000	3.250107	0.000000	0.000000	3.265643
O	0.000000	0.000000	4.398484	0.000000	0.000000	4.434940
C	0.000000	0.000000	-3.250107	0.000000	0.000000	-3.265643
O	0.000000	0.000000	-4.398484	0.000000	0.000000	-4.434940

Table S23 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CO)_2$ **2CO-3S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	2.551504	0.684649	1.049971	2.615627	0.692031	1.028178
C	2.172123	1.163449	-0.280617	2.194187	1.173752	-0.300299
C	1.965985	0.000000	-1.089946	1.959371	0.000000	-1.114467
C	2.172123	-1.163449	-0.280617	2.194187	-1.173752	-0.300299
C	2.551504	-0.684649	1.049971	2.615627	-0.692031	1.028178
H	2.502379	2.113123	-0.691231	2.515430	2.132513	-0.723836
H	1.904351	0.000000	-2.172805	1.877155	0.000000	-2.205957
H	2.764585	1.324984	1.899568	2.854713	1.339830	1.877918
H	2.502379	-2.113123	-0.691231	2.515430	-2.132513	-0.723836
H	2.764585	-1.324984	1.899568	2.854713	-1.339830	1.877918
C	-2.551504	0.684649	1.049971	-2.615627	0.692031	1.028178
C	-2.172123	1.163449	-0.280617	-2.194187	1.173752	-0.300299
C	-1.965985	0.000000	-1.089946	-1.959371	0.000000	-1.114467
C	-2.172123	-1.163449	-0.280617	-2.194187	-1.173752	-0.300299
C	-2.551504	-0.684649	1.049971	-2.615627	-0.692031	1.028178
H	-2.502379	2.113123	-0.691231	-2.515430	2.132513	-0.723836
H	-1.904351	0.000000	-2.172805	-1.877155	0.000000	-2.205957
H	-2.764585	1.324984	1.899568	-2.854713	1.339830	1.877918
H	-2.502379	-2.113123	-0.691231	-2.515430	-2.132513	-0.723836
H	-2.764585	-1.324984	1.899568	-2.854713	-1.339830	1.877918
Pd	0.000000	1.352706	-0.195519	0.000000	1.376256	-0.199222
Pd	0.000000	-1.352706	-0.195519	0.000000	-1.376256	-0.199222
C	0.000000	3.193767	0.257685	0.000000	3.197276	0.300537
C	0.000000	-3.193767	0.257685	0.000000	-3.197276	0.300537
O	0.000000	4.300461	0.563913	0.000000	4.312555	0.651378
O	0.000000	-4.300461	0.563913	0.000000	-4.312555	0.651378

Table S24 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CO)_2$ **2CO-4S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	-2.742213	-1.488660	0.607864	-2.715540	-1.540816	0.652674
C	-3.263528	-0.904915	-0.606555	-3.261308	-0.952698	-0.563494
C	-3.426823	0.468916	-0.371710	-3.443937	0.432843	-0.315488
C	-3.061945	0.732783	1.010917	-3.063259	0.695269	1.075893
C	-2.722126	-0.486617	1.626774	-2.684889	-0.532015	1.682861
H	-2.517890	-2.540208	0.748259	-2.467520	-2.598509	0.784532
H	-3.451263	-1.431996	-1.533875	-3.462404	-1.483286	-1.497625
H	-3.790928	1.204033	-1.080134	-3.837975	1.171631	-1.019445
H	-3.115620	1.701399	1.495560	-3.120650	1.669609	1.570721
H	-2.409796	-0.626433	2.654021	-2.342766	-0.672206	2.711058
C	1.043770	1.705167	-1.334327	1.090052	1.668128	-1.309743
C	2.140925	2.036104	-0.534550	2.127110	2.084171	-0.437960
C	1.637808	2.412913	0.776680	1.505399	2.571600	0.793195
C	0.258594	2.353526	0.760507	0.118271	2.494707	0.665402
C	-0.188512	1.884444	-0.548955	-0.215734	1.904071	-0.637248
H	1.067594	1.489203	-2.396844	1.198206	1.411446	-2.368638
H	3.174174	2.092548	-0.858685	3.189936	2.153529	-0.689909
H	2.256272	2.696928	1.621596	2.053637	2.931637	1.670186
H	-0.398694	2.604588	1.585059	-0.613240	2.812862	1.414175
H	-1.063157	2.323476	-1.031217	-1.068053	2.271936	-1.229652
Pd	1.613219	-0.159954	-0.011392	1.651468	-0.161873	-0.011524
Pd	-1.135820	-0.027982	-0.158016	-1.130074	-0.042495	-0.179668
C	0.197843	-1.405721	-0.691567	0.206536	-1.361497	-0.798964
C	2.939825	-1.352281	0.646541	2.893590	-1.387636	0.738156
O	3.718252	-2.114406	1.012458	3.641220	-2.189071	1.146823
O	0.207651	-2.460898	-1.195043	0.252404	-2.401489	-1.374606

Table S25 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-1S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	1.750318	-1.250747	0.000000	1.745362	-1.258944	0.000000
C	2.113947	-0.498182	1.164124	2.133524	-0.505375	1.174682
C	2.727760	0.734677	0.687499	2.778207	0.723621	0.694887
C	2.727760	0.734677	-0.687499	2.778207	0.723621	-0.694887
C	2.113947	-0.498182	-1.164124	2.133524	-0.505375	-1.174682
H	2.357077	-0.958883	2.116627	2.375275	-0.977646	2.133555
H	3.088420	1.533966	1.327137	3.158672	1.521362	1.342012
H	1.478089	-2.301089	0.000000	1.459583	-2.316011	0.000000
H	3.088420	1.533966	-1.327137	3.158672	1.521362	-1.342012
H	2.357077	-0.958883	-2.116627	2.375275	-0.977646	-2.133555
C	-2.726971	-0.739369	0.687508	-2.776658	-0.735099	0.694901
C	-2.114015	0.493902	1.164120	-2.134380	0.495152	1.174651
C	-1.751009	1.246717	0.000000	-1.747976	1.249528	0.000000
C	-2.114015	0.493902	-1.164120	-2.134380	0.495152	-1.174651
C	-2.726971	-0.739369	-0.687508	-2.776658	-0.735099	-0.694901
H	-2.357268	0.954283	2.116754	-2.376756	0.966747	2.133709
H	-1.479279	2.297188	0.000000	-1.463703	2.306995	0.000000
H	-3.087069	-1.538930	1.327121	-3.155449	-1.533640	1.342016
H	-2.357268	0.954283	-2.116754	-2.376756	0.966747	-2.133709
H	-3.087069	-1.538930	-1.327121	-3.155449	-1.533640	-1.342016
Pd	0.000138	-0.001633	1.346213	0.000091	-0.003531	1.370192
Pd	0.000138	-0.001633	-1.346213	0.000091	-0.003531	-1.370192
C	0.000406	0.001610	3.291035	0.000825	0.003957	3.302346
C	0.000406	0.001610	-3.291035	0.000825	0.003957	-3.302346
N	0.000126	0.005125	-4.467493	0.000559	0.011516	-4.498009
N	0.000126	0.005125	4.467493	0.000559	0.011516	4.498009
C	-0.001114	0.011351	5.879354	-0.000702	0.025827	5.918286
H	0.929747	-0.422738	6.256079	0.893832	-0.494362	6.306815
H	-0.090548	1.037633	6.248009	0.004421	1.067256	6.289142
H	-0.844994	-0.575970	6.253245	-0.903088	-0.483645	6.302719
C	-0.001114	0.011351	-5.879354	-0.000702	0.025827	-5.918286
H	-0.844994	-0.575970	-6.253245	-0.903088	-0.483645	-6.302719
H	0.929747	-0.422738	-6.256079	0.893832	-0.494362	-6.306815
H	-0.090548	1.037633	-6.248009	0.004421	1.067256	-6.289142

Table S26 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-2S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	0.171080	-2.887113	1.916160	0.239891	-2.909406	1.967576
C	1.427844	-2.895741	1.270761	1.481481	-2.918620	1.264358
C	1.236909	-3.325453	-0.091495	1.232023	-3.342666	-0.103113
C	-0.148844	-3.562481	-0.283943	-0.177436	-3.573900	-0.240380
C	-0.814156	-3.232559	0.947885	-0.793916	-3.254807	1.034228
H	-0.020521	-2.596836	2.942003	0.090263	-2.613845	3.009358
H	2.382443	-2.652959	1.722967	2.462620	-2.672532	1.680682
H	2.020322	-3.477897	-0.824197	1.990675	-3.498538	-0.874874
H	-0.614613	-3.945886	-1.183820	-0.685434	-3.960250	-1.128162
H	-1.878856	-3.320719	1.132979	-1.861461	-3.332951	1.261615
C	0.814156	3.232559	0.947885	0.793916	3.254807	1.034228
C	-0.171080	2.887113	1.916160	-0.239891	2.909406	1.967576
C	-1.427844	2.895741	1.270761	-1.481481	2.918620	1.264358
C	-1.236909	3.325453	-0.091495	-1.232023	3.342666	-0.103113
C	0.148844	3.562481	-0.283943	0.177436	3.573900	-0.240380
H	1.878856	3.320719	1.132979	1.861461	3.332951	1.261615
H	0.020521	2.596836	2.942003	-0.090263	2.613845	3.009358
H	-2.382443	2.652959	1.722967	-2.462620	2.672532	1.680682
H	-2.020322	3.477897	-0.824197	-1.990675	3.498538	-0.874874
H	0.614613	3.945886	-1.183820	0.685434	3.960250	-1.128162
Pd	-0.171080	1.300485	0.012035	-0.177436	1.306670	0.016680
Pd	0.171080	-1.300485	0.012035	0.177436	-1.306670	0.016680
C	-1.359811	-0.141634	-0.638311	-1.355288	-0.150614	-0.669323
C	1.359811	0.141634	-0.638311	1.355288	0.150614	-0.669323
N	2.449936	0.252722	-1.163286	2.453968	0.254440	-1.223622
N	-2.449936	-0.252722	-1.163286	-2.453968	-0.254440	-1.223622
C	3.241166	1.361554	-1.617587	3.223243	1.388419	-1.698096
H	4.181045	1.390268	-1.057282	4.186654	1.431353	-1.157620
H	2.711741	2.314078	-1.489226	2.678407	2.342272	-1.552051
H	3.486808	1.222201	-2.674868	3.447145	1.256096	-2.772370
C	-3.241166	-1.361554	-1.617587	-3.223243	-1.388419	-1.698096
H	-3.486808	-1.222201	-2.674868	-3.447145	-1.256096	-2.772370
H	-2.711741	-2.314078	-1.489226	-2.678407	-2.342272	-1.552051
H	-4.181045	-1.390268	-1.057282	-4.186654	-1.431353	-1.157620

Table S27 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-3S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	-2.170485	-1.165200	-0.379245	2.191684	1.176669	-0.415273
C	-1.958404	0.000274	-1.185080	1.948311	0.000593	-1.224615
C	-2.170485	1.165528	-0.378949	2.192970	-1.174886	-0.414829
C	-2.576549	0.685144	0.941844	2.648607	-0.690974	0.900691
C	-2.576565	-0.685151	0.941671	2.647865	0.693742	0.900432
H	-1.883638	0.000401	-2.267323	1.850829	0.000355	-2.315108
H	-2.486936	2.119032	-0.792203	2.501024	-2.136450	-0.842760
H	-2.487045	-2.118530	-0.792826	2.498880	2.138301	-0.843682
H	-2.794096	1.323711	1.792328	2.896508	-1.336856	1.750161
H	-2.794080	-1.323926	1.792009	2.895027	1.340196	1.749684
C	2.170485	-1.165528	-0.378949	-2.192970	1.174886	-0.414829
C	1.958404	-0.000274	-1.185080	-1.948311	-0.000593	-1.224615
C	2.170485	1.165200	-0.379245	-2.191684	-1.176669	-0.415273
C	2.576565	0.685151	0.941671	-2.647865	-0.693742	0.900432
C	2.576549	-0.685144	0.941844	-2.648607	0.690974	0.900691
H	1.883638	-0.000401	-2.267323	-1.850829	-0.000355	-2.315108
H	2.487045	2.118530	-0.792826	-2.498880	-2.138301	-0.843682
H	2.486936	-2.119032	-0.792203	-2.501024	2.136450	-0.842760
H	2.794080	1.323926	1.792009	-2.895027	-1.340196	1.749684
H	2.794096	-1.323711	1.792328	-2.896508	1.336856	1.750161
Pd	0.000022	1.346802	-0.291073	0.000695	-1.369237	-0.307388
Pd	-0.000022	-1.346802	-0.291073	-0.000695	1.369237	-0.307388
C	-0.000564	-3.219182	0.208771	-0.001061	3.212730	0.246910
C	0.000564	3.219182	0.208771	0.001061	-3.212730	0.246910
N	0.001256	4.346036	0.545567	0.001061	-4.344185	0.632003
N	-0.001256	-4.346036	0.545567	-0.001061	4.344185	0.632003
C	0.002795	5.696262	0.957705	0.000059	-5.685555	1.098284
H	0.940405	5.929095	1.471084	-0.950302	-5.909281	1.616496
H	-0.098708	6.350988	0.087039	0.114133	-6.382918	0.248260
H	-0.832661	5.879155	1.639951	0.836416	-5.845049	1.803160
C	-0.002795	-5.696262	0.957705	-0.000059	5.685555	1.098284
H	0.098708	-6.350988	0.087039	-0.114133	6.382918	0.248260
H	-0.940405	-5.929095	1.471084	0.950302	5.909281	1.616496
H	0.832661	-5.879155	1.639951	-0.836416	5.845049	1.803160

Table S28 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-4S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	3.410759	-0.708841	-0.072700	3.415891	-0.724151	-0.016229
C	2.962439	-1.146934	1.222016	2.970963	-1.157595	1.294832
C	2.740152	-0.003500	2.030613	2.745657	0.000870	2.102739
C	2.963499	1.143778	1.228203	2.976341	1.154802	1.289486
C	3.410982	0.712119	-0.068991	3.419636	0.713618	-0.019357
H	3.753785	-1.343470	-0.880976	3.765816	-1.369129	-0.826823
H	2.872454	-2.179102	1.541249	2.869833	-2.197540	1.619487
H	2.390956	-0.006089	3.056026	2.384167	0.004076	3.134563
H	2.873858	2.174378	1.552565	2.880240	2.196610	1.609677
H	3.754194	1.350817	-0.873980	3.772250	1.353319	-0.832946
C	-3.530529	-0.825559	-0.238846	-3.555789	-0.779451	-0.256364
C	-3.588876	0.578603	-0.410165	-3.589995	0.648922	-0.345794
C	-3.216309	1.180145	0.844146	-3.225754	1.175919	0.959077
C	-3.026727	0.147351	1.804547	-3.042959	0.077217	1.860855
C	-3.156377	-1.088718	1.130291	-3.186127	-1.128348	1.106955
H	-3.746546	-1.574481	-0.991239	-3.783873	-1.485643	-1.059119
H	-3.853828	1.108083	-1.317082	-3.848487	1.239461	-1.228582
H	-3.162660	2.245820	1.035341	-3.154609	2.237498	1.213797
H	-2.746457	0.284980	2.841709	-2.755965	0.149444	2.913135
H	-3.038257	-2.073029	1.568524	-3.074826	-2.146991	1.489957
Pd	-1.399917	-0.000254	-0.040906	-1.404258	0.001778	-0.039050
Pd	1.222531	0.000683	0.052348	1.229276	-0.000120	0.057312
C	-0.080659	-1.366862	-0.642435	-0.077699	-1.358608	-0.685569
C	-0.080341	1.368452	-0.638651	-0.075743	1.361751	-0.683443
N	-0.101065	-2.466014	-1.159952	-0.115041	-2.459064	-1.244854
N	-0.104650	2.467724	-1.155439	-0.110421	2.462390	-1.242229
C	0.893607	3.412124	-1.571291	0.913298	3.388249	-1.686121
H	1.907703	3.038315	-1.381614	1.932212	3.005833	-1.477054
H	0.748117	4.354220	-1.033537	0.776412	4.359510	-1.176390
H	0.775783	3.616194	-2.640073	0.804080	3.561727	-2.772357
C	0.900817	-3.407860	-1.572980	0.906955	-3.386975	-1.688555
H	1.913437	-3.031132	-1.381266	1.926663	-3.006231	-1.480407
H	0.756673	-4.349980	-1.034885	0.768634	-4.357568	-1.177910
H	0.785962	-3.613004	-2.641885	0.796794	-3.561230	-2.774576

Table S29 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CS)_2$ **2CS-1S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	0.000000	2.918393	1.868225	0.000000	2.967769	1.893139
H	0.000000	2.632063	2.912909	0.000000	2.687426	2.949830
C	1.146507	3.092512	1.049291	1.157487	3.137181	1.066359
H	2.178707	3.004091	1.367423	2.198943	3.046681	1.387903
C	0.710038	3.464542	-0.269818	0.718046	3.487587	-0.270461
H	1.352052	3.706250	-1.108136	1.365260	3.721745	-1.119783
C	-0.710038	3.464542	-0.269818	-0.718046	3.487587	-0.270461
H	-1.352052	3.706250	-1.108136	-1.365260	3.721745	-1.119783
C	-1.146507	3.092512	1.049291	-1.157487	3.137181	1.066359
H	-2.178707	3.004091	1.367423	-2.198943	3.046681	1.387903
C	0.000000	-2.918393	1.868225	0.000000	-2.967769	1.893139
H	0.000000	-2.632063	2.912909	0.000000	-2.687426	2.949830
C	1.146507	-3.092512	1.049291	1.157487	-3.137181	1.066359
H	2.178707	-3.004091	1.367423	2.198943	-3.046681	1.387903
C	0.710038	-3.464542	-0.269818	0.718046	-3.487587	-0.270461
H	1.352052	-3.706250	-1.108136	1.365260	-3.721745	-1.119783
C	-0.710038	-3.464542	-0.269818	-0.718046	-3.487587	-0.270461
H	-1.352052	-3.706250	-1.108136	-1.365260	-3.721745	-1.119783
C	-1.146507	-3.092512	1.049291	-1.157487	-3.137181	1.066359
H	-2.178707	-3.004091	1.367423	-2.198943	-3.046681	1.387903
Pd	0.000000	1.307392	0.020475	0.000000	1.318437	0.016708
Pd	0.000000	-1.307392	0.020475	0.000000	-1.318437	0.016708
C	1.334660	0.000000	-0.630928	1.345156	0.000000	-0.639442
C	-1.334660	0.000000	-0.630928	-1.345156	0.000000	-0.639442
S	2.748498	0.000000	-1.321924	2.782063	0.000000	-1.332976
S	-2.748498	0.000000	-1.321924	-2.782063	0.000000	-1.332976

Table S30 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CS)_2$ **2CS-2S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	-2.679494	-1.690348	0.746746	-2.490541	-1.869231	0.841231
C	-3.340261	-1.174916	-0.430079	-3.283573	-1.340578	-0.255304
C	-3.699456	0.155610	-0.156667	-3.662827	-0.016352	0.104384
C	-3.314346	0.452797	1.207865	-3.172175	0.246540	1.456229
C	-2.759246	-0.705918	1.781687	-2.500908	-0.910666	1.924460
H	-2.290862	-2.696500	0.854985	-2.043996	-2.867537	0.874894
H	-3.491380	-1.711274	-1.358722	-3.512003	-1.855818	-1.191537
H	-4.199318	0.837096	-0.835677	-4.262761	0.670353	-0.500455
H	-3.480226	1.398805	1.711731	-3.326632	1.174124	2.015344
H	-2.377008	-0.809195	2.789560	-2.001066	-1.028690	2.889201
C	0.453774	2.015502	-1.499624	0.467265	1.941695	-1.455899
C	1.590484	2.513660	-0.860568	1.405409	2.639751	-0.652571
C	1.237592	2.801676	0.517799	0.714814	3.085925	0.553564
C	-0.113486	2.529882	0.696493	-0.626755	2.705824	0.477626
C	-0.661617	2.003347	-0.544889	-0.846310	1.947384	-0.758664
H	0.371341	1.755003	-2.548580	0.609715	1.629638	-2.495548
H	2.558435	2.685377	-1.317431	2.426915	2.905814	-0.941907
H	1.916438	3.188316	1.270100	1.187069	3.624468	1.381920
H	-0.677344	2.678389	1.610008	-1.398072	2.923848	1.222225
H	-1.665973	2.262119	-0.880496	-1.771959	2.056122	-1.344848
Pd	1.386861	0.339269	-0.043033	1.438025	0.362613	-0.074132
Pd	-1.321279	-0.053444	-0.075601	-1.297897	-0.112508	-0.100581
C	0.200051	-1.152852	-0.619254	0.232420	-1.072452	-0.837886
C	2.861515	-0.636123	0.565306	2.856009	-0.589083	0.722923
S	0.444516	-2.559483	-1.295073	0.563528	-2.356205	-1.727542
S	4.034611	-1.528641	1.028371	4.004594	-1.478149	1.315476

Table S31 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CS)_2$ **2CS-3S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	1.341094	2.481696	0.687209	1.344222	2.529887	0.694922
C	0.000000	2.169174	1.163782	0.000000	2.189329	1.174026
C	-0.815007	1.970077	0.000000	-0.822124	1.968242	0.000000
C	0.000000	2.169174	-1.163782	0.000000	2.189329	-1.174026
C	1.341094	2.481696	-0.687209	1.344222	2.529887	-0.694922
H	-0.394878	2.518937	2.112085	-0.405076	2.536273	2.130749
H	-1.899710	1.949107	0.000000	-1.916459	1.935628	0.000000
H	2.197882	2.661718	1.327950	2.203873	2.729766	1.342867
H	-0.394878	2.518937	-2.112085	-0.405076	2.536273	-2.130749
H	2.197882	2.661718	-1.327950	2.203873	2.729766	-1.342867
C	0.815007	-1.970077	0.000000	0.822124	-1.968242	0.000000
C	0.000000	-2.169174	1.163782	0.000000	-2.189329	1.174026
C	-1.341094	-2.481696	0.687209	-1.344222	-2.529887	0.694922
C	-1.341094	-2.481696	-0.687209	-1.344222	-2.529887	-0.694922
C	0.000000	-2.169174	-1.163782	0.000000	-2.189329	-1.174026
H	0.394878	-2.518937	2.112085	0.405076	-2.536273	2.130749
H	-2.197882	-2.661718	1.327950	-2.203873	-2.729766	1.342867
H	1.899710	-1.949107	0.000000	1.916459	-1.935628	0.000000
H	-2.197882	-2.661718	-1.327950	-2.203873	-2.729766	-1.342867
H	0.394878	-2.518937	-2.112085	0.405076	-2.536273	-2.130749
Pd	0.000000	0.000000	1.377953	0.000000	0.000000	1.406655
Pd	0.000000	0.000000	-1.377953	0.000000	0.000000	-1.406655
C	0.000000	0.000000	3.250890	0.000000	0.000000	3.279518
C	0.000000	0.000000	-3.250890	0.000000	0.000000	-3.279518
S	0.000000	0.000000	4.797031	0.000000	0.000000	4.848606
S	0.000000	0.000000	-4.797031	0.000000	0.000000	-4.848606

Table S32 Theoretical cartesian coordinates (in Å) of $Cp_2Pd_2(CS)_2$ **2CS-4S** using the MPW1PW91 and BP86 methods

Atom	MPW1PW91			BP86		
	X	Y	Z	X	Y	Z
C	2.602730	0.684522	0.898505	2.688174	0.692084	0.821642
C	2.165134	1.165048	-0.411998	2.184177	1.175294	-0.474778
C	1.918344	0.000000	-1.211864	1.895212	0.000000	-1.273887
C	2.165134	-1.165048	-0.411998	2.184177	-1.175294	-0.474778
C	2.602730	-0.684522	0.898505	2.688174	-0.692084	0.821642
H	2.476280	2.115506	-0.834963	2.475482	2.136089	-0.914924
H	1.822302	0.000000	-2.292421	1.761965	0.000000	-2.360586
H	2.850054	1.325196	1.738436	2.975822	1.340110	1.655907
H	2.476280	-2.115506	-0.834963	2.475482	-2.136089	-0.914924
H	2.850054	-1.325196	1.738436	2.975822	-1.340110	1.655907
C	-2.602730	0.684522	0.898505	-2.688174	0.692084	0.821642
C	-2.165134	1.165048	-0.411998	-2.184177	1.175294	-0.474778
C	-1.918344	0.000000	-1.211864	-1.895212	0.000000	-1.273887
C	-2.165134	-1.165048	-0.411998	-2.184177	-1.175294	-0.474778
C	-2.602730	-0.684522	0.898505	-2.688174	-0.692084	0.821642
H	-2.476280	2.115506	-0.834963	-2.475482	2.136089	-0.914924
H	-1.822302	0.000000	-2.292421	-1.761965	0.000000	-2.360586
H	-2.850054	1.325196	1.738436	-2.975822	1.340110	1.655907
H	-2.476280	-2.115506	-0.834963	-2.475482	-2.136089	-0.914924
H	-2.850054	-1.325196	1.738436	-2.975822	-1.340110	1.655907
Pd	0.000000	1.378439	-0.279643	0.000000	1.404028	-0.294777
Pd	0.000000	-1.378439	-0.279643	0.000000	-1.404028	-0.294777
C	0.000000	3.159578	0.282073	0.000000	3.154368	0.355337
C	0.000000	-3.159578	0.282073	0.000000	-3.154368	0.355337
S	0.000000	4.609288	0.818107	0.000000	4.590084	0.986704
S	0.000000	-4.609288	0.818107	0.000000	-4.590084	0.986704

Table S33 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2F_2$ **2F-1S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
29(0), 70(3), 82(2), 120(1), 128(0), 141(1), 158(0), 170(3), 187(4), 242(0), 283(17), 340(0), 347(2), 360(3), 416(2), 453(12), 528(97), 566(8), 596(0), 614(2), 633(0), 744(4), 756(13), 771(17), 782(88), 809(21), 821(8), 830(1), 831(1), 836(3), 884(1), 891(2), 908(11), 931(9), 946(0), 1001(8), 1009(14), 1024(16), 1043(22), 1060(1), 1069(2), 1082(19), 1086(1), 1126(4), 1158(68), 1270(0), 1276(0), 1308(2), 1337(31), 1378(22), 1392(9), 1403(13), 1444(4), 1458(33), 1466(7), 1500(1), 3042(29), 3218(2), 3223(1), 3246(1), 3258(1), 3264(1), 3269(0), 3272(1), 3285(1), 3292(2)	28(0), 65(3), 83(2), 113(1), 122(1), 134(1), 152(0), 165(3), 183(3), 232(0), 270(12), 328(0), 336(2), 348(1), 390(1), 438(7), 505(74), 537(10), 564(0), 580(1), 598(0), 704(3), 722(13), 736(18), 746(73), 767(15), 785(6), 791(2), 795(2), 801(2), 833(0), 841(2), 864(13), 877(5), 891(1), 955(8), 966(13), 982(14), 991(20), 1020(1), 1024(25), 1033(18), 1040(0), 1074(3), 1079(46), 1216(0), 1220(0), 1237(2), 1274(32), 1310(13), 1326(6), 1334(12), 1372(28), 1379(4), 1396(1), 1414(1), 2919(37), 3109(1), 3110(4), 3130(2), 3144(0), 3152(1), 3157(0), 3158(1), 3175(1), 3183(2)

Table S34 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2F_2$ **2F-2S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
35(0), 80(0), 86(22), 103(1), 131(10), 133(14), 152(0), 182(0), 185(14), 208(2), 248(0), 251(15), 354(20), 370(2), 388(15), 393(0), 469(223), 509(0), 587(2), 600(0), 608(2), 624(0), 788(3), 791(115), 800(0), 802(0), 816(126), 818(0), 820(1), 839(1), 848(2), 870(2), 873(2), 907(0), 912(0), 918(3), 980(20), 990(14), 1027(0), 1027(22), 1060(30), 1062(0), 1075(1), 1083(0), 1114(4), 1117(0), 1273(0), 1274(0), 1347(0), 1355(59), 1393(4), 1435(0), 1443(24), 1443(23), 1460(0), 1464(13), 3267(0), 3267(0), 3267(0), 3267(1), 3277(1), 3277(1), 3280(0), 3280(23), 3288(0), 3288(0)	29(0), 65(0), 70(17), 97(0), 117(4), 130(13), 147(0), 177(0), 177(1), 182(10), 222(7), 224(0), 353(0), 354(8), 355(8), 366(2), 459(183), 487(0), 562(0), 564(2), 570(1), 591(0), 752(149), 758(1), 759(3), 761(0), 780(0), 783(0), 784(49), 800(2), 808(5), 828(3), 831(0), 855(0), 857(0), 862(5), 939(12), 943(12), 983(0), 984(18), 1023(16), 1026(1), 1034(1), 1045(0), 1064(1), 1066(0), 1220(0), 1221(0), 1290(29), 1295(2), 1319(2), 1367(0), 1378(20), 1378(19), 1395(0), 1397(11), 3149(0), 3150(0), 3155(0), 3155(1), 3161(1), 3161(0), 3169(0), 3169(9), 3177(0), 3177(0)

Table S35 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2F_2$ **2F-3S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
24(3), 55(0), 70(4), 90(0), 105(0), 115(0), 119(0), 143(0), 158(2), 171(2), 296(6), 301(0), 340(4), 348(1), 372(0), 403(21), 422(0), 437(501), 540(0), 541(2), 602(14), 602(0), 725(79), 726(0), 786(82), 787(6), 806(0), 806(1), 828(56), 829(0), 888(0), 889(0), 912(0), 913(20), 932(8), 933(2), 962(0), 962(15), 1026(11), 1027(19), 1061(0), 1061(1), 1072(1), 1073(13), 1139(3), 1139(0), 1272(0), 1272(0), 1371(0), 1371(9), 1419(36), 1420(1), 1433(0), 1433(16), 1575(22), 1576(5), 3265(1), 3265(2), 3266(0), 3266(3), 3278(0), 3278(2), 3292(0), 3292(0), 3299(2), 3299(1)	26(3), 50(0), 66(4), 88(0), 101(0), 111(0), 115(0), 160(0), 169(2), 180(5), 280(5), 282(0), 337(10), 344(1), 359(0), 381(17), 413(0), 423(361), 517(0), 518(2), 572(15), 573(1), 680(84), 680(0), 745(50), 747(8), 771(0), 772(1), 784(45), 785(0), 841(0), 841(0), 860(0), 860(20), 877(6), 879(4), 911(0), 911(11), 982(11), 982(16), 1017(0), 1018(1), 1027(0), 1028(12), 1090(5), 1090(0), 1218(0), 1218(0), 1299(0), 1299(8), 1347(36), 1348(1), 1359(0), 1360(17), 1512(23), 1513(4), 3150(2), 3150(2), 3151(0), 3151(6), 3165(0), 3165(6), 3175(1), 3176(2), 3186(4), 3186(2)

Table S36 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2F_2$ **2F-4S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
34(1), 42(0), 83(2), 103(2), 110(1), 134(2), 163(2), 166(3), 191(2), 199(6), 222(3), 238(3), 329(2), 345(5), 397(24), 403(9), 446(26), 542(3), 578(140), 590(2), 593(13), 690(9), 752(8), 771(69), 777(94), 805(10), 810(3), 817(1), 839(24), 851(41), 888(3), 906(14), 916(10), 925(1), 933(3), 940(44), 987(6), 989(9), 1022(5), 1033(12), 1064(13), 1066(7), 1082(4), 1087(0), 1126(3), 1144(0), 1275(1), 1277(0), 1335(2), 1377(3), 1408(52), 1411(19), 1433(55), 1469(21), 1529(2), 1568(43), 3172(2), 3238(2), 3253(5), 3262(1), 3261(2), 3277(0), 3281(4), 3285(0), 3297(0), 3304(1)	31(0), 41(0), 72(4), 96(1), 102(1), 124(2), 139(1), 155(3), 184(4), 185(2), 215(6), 220(1), 319(5), 323(2), 372(22), 402(2), 420(8), 511(4), 554(8), 556(109), 562(10), 655(3), 712(7), 729(74), 739(92), 766(7), 779(1), 785(3), 804(17), 815(29), 833(7), 852(3), 859(10), 864(8), 877(5), 906(12), 945(2), 950(8), 972(2), 989(12), 1024(11), 1028(3), 1039(2), 1039(2), 1077(4), 1096(0), 1221(1), 1223(0), 1267(2), 1311(4), 1340(63), 1353(25), 1353(6), 1395(18), 1454(2), 1470(36), 3058(2), 3122(2), 3135(8), 3151(2), 3151(3), 3167(0), 3170(4), 3175(1), 3187(0), 3193(1)

Table S37 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2F_2$ **2Cl-1S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
33(0), 55(12), 69(0), 98(6), 99(2), 121(5), 131(0), 171(0), 173(30), 207(2), 210(0), 249(12), 299(88), 342(0), 345(17), 362(2), 391(1), 394(0), 584(1), 598(0), 608(1), 622(0), 789(0), 796(85), 806(0), 810(0), 815(176), 819(0), 822(0), 838(1), 848(0), 870(1), 878(2), 910(1), 912(0), 919(2), 985(24), 995(13), 1026(0), 1026(13), 1061(23), 1063(0), 1077(0), 1084(0), 1114(6), 1117(0), 1273(0), 1274(0), 1345(0), 1353(57), 1395(5), 1435(0), 1440(25), 1442(23), 1460(0), 1464(17), 3269(0), 3270(1), 3270(0), 3270(0), 3279(1), 3280(4), 3282(0), 3282(20), 3290(1), 3290(0)	30(0), 45(10), 57(0), 95(6), 95(1), 113(3), 125(0), 167(0), 170(20), 178(1), 193(0), 222(7), 291(73), 322(0), 344(8), 357(2), 358(0), 360(0), 562(0), 565(2), 567(0), 589(0), 759(144), 761(0), 766(1), 769(0), 783(0), 784(75), 785(0), 801(2), 806(1), 826(1), 836(0), 858(0), 860(0), 865(4), 941(14), 948(11), 983(0), 984(11), 1023(12), 1027(1), 1036(0), 1046(0), 1064(3), 1067(0), 1220(0), 1221(0), 1289(29), 1294(1), 1322(3), 1367(0), 1377(21), 1377(20), 1395(0), 1398(15), 3155(0), 3155(0), 3158(0), 3158(1), 3165(1), 3165(0), 3171(0), 3171(6), 3178(0), 3179(0)

Table S38 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2F_2$ **2Cl-2S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
12(2), 45(0), 66(3), 73(1), 78(0), 87(0), 103(0), 107(0), 1281), 139(0), 251(0), 262(12), 270(56), 271(1), 290(0), 294(2), 340(58), 342(0), 527(0), 527(2), 591(27), 592(0), 729(65), 730(0), 776(102), 776(11), 803(0), 801(1), 832(89), 833(0), 885(0), 885(1), 909(0), 909(10), 924(7), 924(0), 967(0), 968(11), 1031(23), 1033(27), 1061(0), 1062(0), 1073(8), 1073(11), 1141(2), 1141(0), 1273(0), 1273(0), 1369(0), 1369(7), 1425(67), 1426(4), 1432(0), 1432(28), 1561(40), 1562(7), 3270(2), 3271(1), 3271(0), 3271(2), 3283(0), 3283(1), 3297(0), 3298(0), 3304(3), 3304(0)	19(2), 51(0), 60(2), 80(0), 82(2), 83(0), 101(0), 119(0), 123(0), 137(0), 233(0), 249(10), 256(39), 271(0), 271(2), 271(1), 330(29), 334(0), 507(2), 507(0), 562(31), 563(1), 684(74), 684(1), 739(60), 740(20), 771(0), 771(1), 791(73), 792(1), 837(0), 837(1), 854(0), 855(11), 871(6), 871(2), 918(0), 918(9), 986(18), 988(24), 1020(0), 1020(0), 1029(8), 1030(10), 1091(3), 1092(0), 1220(0), 1220(0), 1299(7), 1299(0), 1354(62), 1355(5), 1365(0), 1365(25), 1499(36), 1500(8), 3156(2), 3156(2), 3157(0), 3157(4), 3169(0), 3169(5), 3183(0), 3183(1), 3190(6), 3190(0)

Table S39 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2Cl_2$ **2Cl-3S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
40(0), 55(2), 67(0), 100(0), 111(0), 121(1), 135(0), 147(2), 185(6), 224(1), 281(8), 285(7), 324(7), 341(34), 357(1), 408(2), 421(0), 444(4), 601(0), 609(2), 632(1), 734(17), 741(3), 773(4), 780(110), 814(15), 814(14), 826(5), 830(3), 834(4), 844(38), 888(1), 893(3), 923(8), 946(0), 963(9), 1008(13), 1020(8), 1024(14), 1037(13), 1059(2), 1071(2), 1088(2), 1101(9), 1125(5), 1241(31), 1265(3), 1269(0), 1291(5), 1374(8), 1388(9), 1403(10), 1442(5), 1448(15), 1470(4), 1494(2), 3081(7), 3216(2), 3229(0), 3246(1), 3263(1), 3266(1), 3271(0), 3275(1), 3287(0), 3293(2)	22(0), 54(2), 63(0), 97(0), 105(0), 114(1), 138(0), 143(1), 183(5), 213(0), 268(10), 273(1), 316(13), 329(18), 342(1), 388(1), 410(0), 416(6), 572(0), 577(2), 599(1), 699(16), 701(2), 738(7), 743(98), 772(20), 775(7), 788(6), 795(3), 799(2), 800(30), 837(0), 842(3), 869(9), 946(0), 891(0), 912(8), 966(12), 974(7), 982(14), 988(10), 1019(1), 1031(2), 1043(1), 1054(6), 1075(3), 1181(32), 1210(4), 1217(0), 1225(2), 1308(6), 1321(6), 1334(7), 1362(12), 1377(3), 1399(3), 1406(2), 2965(11), 3109(2), 3114(2), 3130(2), 3148(0), 3156(1), 3160(1), 3161(1), 3178(1), 3184(2)

Table S40 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2Cl_2$ **2Cl-4S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
21(1), 30(0), 80(0), 89(1), 97(1), 111(2), 127(3), 137(4), 176(1), 195(3), 217(2), 244(0), 265(2), 276(13), 318(1), 338(14), 359(48), 396(4), 539(2), 583(2), 587(6), 684(5), 758(7), 776(73), 780(92), 801(5), 807(11), 815(1), 839(23), 848(43), 887(4), 909(9), 918(8), 924(2), 938(3), 959(10), 990(6), 991(4), 1027(8), 1034(11), 1059(6), 1065(13), 1079(3), 1090(0), 1128(4), 1145(0), 1271(0), 1277(0), 1330(2), 1375(4), 1404(28), 1408(26), 1439(35), 1466(26), 1524(2), 1589(25), 3150(9), 3238(3), 3257(4), 3262(2), 3264(1), 3280(0), 3282(4), 3288(0), 3299(1), 3306(0)	11(1), 30(0), 73(1), 76(0), 85(1), 104(1), 114(2), 130(3), 151(1), 183(3), 201(2), 222(2), 244(2), 257(10), 306(0), 312(9), 348(39), 389(1), 507(1), 546(2), 557(4), 645(2), 720(6), 738(77), 743(93), 764(6), 774(5), 783(1), 803(17), 808(20), 829(5), 854(3), 861(2), 861(8), 883(2), 907(2), 950(2), 951(6), 978(3), 992(12), 1020(2), 1025(10), 1037(2), 1041(0), 1081(4), 1097(0), 1219(0), 1224(0), 1268(2), 1309(3), 1338(46), 1345(8), 1355(4), 1392(20), 1450(2), 1498(12), 3041(6), 3124(4), 3143(5), 3150(3), 3152(2), 3170(0), 3171(5), 3178(0), 3189(0), 3196(1)

Table S41 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CN)_2$ **2CN-1S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
40(1), 55(5), 65(3), 85(3), 93(3), 105(1), 122(1), 153(1), 178(5), 201(4), 226(0), 278(12), 289(6), 330(0), 349(2), 368(2), 393(7), 407(2), 443(2), 447(16), 524(2), 547(0), 605(0), 615(2), 631(1), 748(21), 755(8), 782(52), 785(13), 809(38), 818(19), 829(0), 830(4), 839(12), 885(26), 891(4), 900(8), 930(12), 950(0), 1005(11), 1006(8), 1027(15), 1030(15), 1059(1), 1064(2), 1074(1), 1091(2), 1108(13), 1123(6), 1236(7), 1271(0), 1280(2), 1295(5), 1376(4), 1393(4), 1403(7), 1445(3), 1448(12), 1465(6), 1495(0), 2254(8), 2372(11), 3030(3), 3221(1), 3231(0), 3249(1), 3263(1), 3270(0), 3275(2), 3277(3), 3285(0), 3292(2)	23(2), 52(3), 59(3), 79(3), 86(2), 98(1), 121(1), 141(0), 173(4), 190(3), 216(0), 268(9), 273(5), 319(0), 333(1), 356(0), 380(3), 387(2), 416(3), 434(10), 500(1), 518(0), 572(0), 581(1), 596(1), 715(10), 720(10), 749(37), 751(26), 770(40), 779(10), 789(3), 795(1), 802(8), 839(18), 844(12), 852(5), 876(9), 892(1), 965(5), 965(12), 979(14), 984(13), 1014(1), 1022(2), 1034(0), 1045(2), 1061(11), 1071(4), 1170(8), 1218(0), 1219(1), 1234(7), 1310(4), 1324(5), 1335(2), 1360(9), 1382(3), 1390(3), 1407(0), 2116(5), 2240(9), 2900(7), 3115(2), 3116(1), 3134(1), 3150(0), 3161(1), 3164(1), 3167(1), 3175(0), 3183(2)

Table S42 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CN)_2$ **2CN-2S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
16(0), 23(2), 25(1), 36(0), 67(2), 79(0), 104(0), 139(1), 162(0), 164(1), 240(1), 248(0), 306(0), 317(33), 324(1), 329(53), 332(0), 350 (0), 393(0), 413(28), 467(58), 492(0), 555(0), 559(1), 599(10), 600(0), 743(9), 744(4), 774(211), 775(0), 818(0), 820(1), 840(64), 841(0), 881(0), 881(4), 906(0), 907(1), 929(0), 930(7), 988(0), 989(17), 1035(8), 1035(34), 1065(28), 1066(0), 1077(8), 1078(1), 1143(0), 1143(0), 1276(0), 1276(0), 1374(3), 1375(1), 1414(49), 1415(1), 1458(102), 1460(0), 1530(15), 1530(2), 2130(0), 2153(542), 3275(1), 3275(0), 3276(1), 3276(0), 3286(0), 3286(1), 3299(0), 3299(0), 3306(2), 3306(0)	20(2), 26(0), 32(1), 59(0), 66(2), 75(0), 98(1), 128(0), 137(0), 149(1), 218(2), 225(0), 292(0), 305(8), 306(0), 320(10), 323(44), 352(0), 390(0), 414(18), 488(26), 500(0), 519(0), 528(1), 566(0), 567(7), 700(3), 701(5), 734(206), 735(0), 783(0), 788(0), 806(56), 808(0), 828(0), 828(8), 850(0), 850(0), 874(0), 875(4), 948(0), 948(17), 991(33), 992(3), 1026(33), 1026(0), 1035(8), 1036(0), 1096(1), 1096(0), 1222(0), 1222(0), 1305(3), 1308(0), 1349(49), 1349(0), 1393(110), 1395(0), 1456(1), 1456(6), 1981(0), 2004(547), 3163(3), 3163(0), 3166(1), 3166(0), 3176(0), 3176(4), 3190(0), 3190(0), 3196(4), 3196(0)

Table S43 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CN)_2$ **2CN-3S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
28(2), 37(0), 64(2), 68(0), 81(0), 89(1), 97(0), 130(0), 161(1), 189(0), 279(16), 279(2), 285(1), 295(13), 305(2), 313(0), 346(23), 355(3), 375(2), 426(29), 468(7), 495(67), 521(3), 571(1), 592(6), 607(1), 735(28), 754(8), 775(85), 782(98), 803(1), 827(1), 835(46), 845(23), 867(1), 886(0), 904(1), 911(4), 914(4), 925(3), 973(8), 995(9), 1034(29), 1042(27), 1061(0), 1067(0), 1073(14), 1073(8), 1141(1), 1145(0), 1274(0), 1274(0), 1369(2), 1384(1), 1423(84), 1427(16), 1434(12), 1443(11), 1518(14), 1552(23), 2174(39), 2197(505), 3273(1), 3274(1), 3276(1), 3277(1), 3284(0), 3287(1), 3298(0), 3299(0), 3305(1), 3306(2)	28(2), 36(0), 61(2), 65(0), 79(0), 91(0), 97(0), 112(2), 160(1), 169(1), 259(1), 262(1), 268(2), 269(4), 290(9), 307(1), 330(8), 339(1), 356(1), 412(37), 454(3), 496(4), 499(32), 536(1), 557(6), 572(0), 689(35), 711(6), 737(68), 743(95), 769(1), 791(1), 798(41), 811(21), 820(1), 834(0), 851(1), 855(4), 859(3), 866(4), 926(6), 953(9), 991(30), 1001(27), 1019(0), 1026(0), 1030(10), 1033(13), 1092(1), 1097(0), 1222(0), 1222(0), 1300(2), 1315(1), 1356(93), 1359(10), 1366(10), 1378(11), 1449(13), 1485(24), 2033(47), 2059(394), 3160(1), 3161(2), 3166(1), 3167(1), 3172(2), 3178(2), 3187(0), 3189(0), 3193(3), 3197(2)

Table S44 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CN)_2$ **2CN-4S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
24(4), 36(1), 50(0), 68(0), 79(2), 98(0), 103(1), 111(1), 143(0), 147(3), 179(0), 237(3), 246(16), 270(12), 302(5), 308(2), 327(3), 338(3), 349(4), 361(3), 422(4), 474(20), 522(1), 557(2), 591(7), 599(1), 742(35), 752(11), 778(122), 781(24), 800(3), 818(2), 836(53), 842(20), 882(2), 898(2), 911(3), 918(3), 923(2), 937(1), 970(4), 988(7), 1037(37), 1041(16), 1063(1), 1065(1), 1075(17), 1076(4), 1143(0), 1144(0), 1276(0), 1277(0), 1365(2), 1374(5), 1421(42), 1425(27), 1441(19), 1445(26), 1529(13), 1558(21), 2118(50), 2162(4), 3277(1), 3277(1), 3280(1), 3280(0), 3288(0), 3290(0), 3301(1), 3301(0), 3308(1), 3308(2)	26(2), 33(2), 39(1), 75(2), 80(1), 95(0), 103(2), 127(0), 131(1), 162(1), 181(9), 217(7), 235(2), 248(12), 282(7), 295(3), 312(14), 320(2), 353(4), 363(6), 403(5), 478(18), 497(1), 530(2), 554(10), 561(0), 705(26), 714(12), 743(86), 746(60), 769(4), 787(14), 804(30), 808(17), 823(2), 840(2), 853(1), 858(2), 864(1), 878(2), 935(5), 952(8), 995(28), 1004(20), 1020(8), 1029(0), 1030(9), 1034(7), 1096(0), 1098(0), 1223(0), 1223(0), 1300(1), 1313(7), 1346(48), 1353(25), 1378(24), 1386(22), 1446(8), 1469(15), 1961(23), 2008(11), 3167(0), 3167(0), 3170(0), 3170(0), 3177(0), 3179(1), 3189(0), 3192(0), 3199(2), 3199(2)

Table S45 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CN)_2$ **2CN-5S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
17(7), 43(0), 46(0), 65(1), 66(2), 73(2), 87(0), 103(1), 126(0), 129(0), 148(2), 158(0), 255(0), 282(0), 303(61), 317(1), 321(0), 325(0), 334(0), 346(2), 365(29), 367(0), 502(0), 528(0), 589(0), 590(3), 744(49), 745(5), 777(136), 778(0), 786(1), 801(0), 836(88), 839(1), 892(0), 892(3), 914(0), 914(2), 927(0), 928(1), 973(12), 974(0), 1038(47), 1040(25), 1058(0), 1062(0), 1073(12), 1074(11), 1142(0), 1142(0), 1276(0), 1276(0), 1354(0), 1361(0), 1429(106), 1429(47), 1431(0), 1432(1), 1546(52), 1548(4), 2145(0), 2151(0), 3279(1), 3279(0), 3279(1), 3279(0), 3289(0), 3289(1), 3302(0), 3302(1), 3308(2), 3308(1)	20(6), 27(0), 48(0), 63(1), 66(1), 77(0), 78(0), 118(0), 119(0), 126(0), 134(0), 141(0), 250(0), 258(0), 289(4), 297(2), 310(0), 314(0), 326(22), 335(2), 348(28), 368(1), 432(0), 501(0), 553(1), 564(2), 689(45), 699(7), 726(6), 736(139), 737(0), 765(0), 801(69), 804(1), 840(0), 840(4), 861(1), 861(0), 871(0), 871(2), 928(14), 930(0), 997(49), 1000(22), 1009(1), 1019(0), 1031(12), 1032(11), 1095(0), 1095(0), 1224(0), 1224(0), 1270(2), 1290(0), 1361(103), 1362(49), 1364(0), 1365(0), 1475(49), 1478(2), 1976(0), 1987(0), 3168(0), 3168(1), 3168(1), 3168(0), 3178(0), 3178(0), 3192(0), 3192(0), 3198(3), 3198(1)

Table S46 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CN)_2$ **2CN-6S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
18(0), 50(0), 51(20), 65(14), 81(0), 103(2), 111(0), 158(45), 160(0), 228(0), 235(6), 270(33), 277(0), 291(0), 301(0), 304(0), 333(4), 355(0), 371(65), 401(0), 421(3), 428(0), 604(0), 605(4), 624(0), 625(1), 793(4), 800(0), 805(0), 806(163), 818(0), 820(2), 829(0), 832(71), 842(0), 846(3), 888(0), 905(2), 911(3), 926(0), 996(15), 996(10), 1026(26), 1031(0), 1053(41), 1064(0), 1074(0), 1081(0), 1117(4), 1119(0), 1273(0), 1273(0), 1341(0), 1369(88), 1401(7), 1424(0), 1425(0), 1434(21), 1463(0), 1466(15), 2248(7), 2250(0), 3273(0), 3273(3), 3275(2), 3276(0), 3283(8), 3283(0), 3288(20), 3288(0), 3299(10), 3299(0)	3(1), 47(17), 49(0), 61(13), 77(0), 983(1), 111(0), 153(0), 154(35), 207(0), 208(5), 251(0), 260(15), 280(0), 284(0), 287(0), 318(2), 339(0), 363(47), 385(0), 399(2), 402(0), 574(2), 577(0), 587(0), 587(1), 761(68), 764(0), 766(46), 767(0), 783(0), 783(4), 784(0), 789(80), 799(1), 802(0), 839(0), 852(2), 857(1), 868(0), 953(15), 953(0), 985 (19), 988(0), 1015(27), 1024(0), 1032(0), 1040(0), 1068(2), 1070(0), 1219(0), 1220(0), 1285(0), 1309(54), 1335(5), 1352(0), 1359(0), 1366(19), 1396(0), 1399(13), 2117(2), 2120(0), 3163(0), 3163(3), 3164(1), 3165(0), 3172(3), 3172(0), 3177(13), 3177(0), 3187(5), 3187(0)

Table S47 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CO)_2$ **2CO-1S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
8(0), 11(0), 26(1), 76(0), 79(0), 80(0), 104(0), 169(0), 176(2), 198(0), 221(17), 228(0), 247(8), 252(0), 292(103), 333(2), 394(1), 428(24), 431(2), 445(0), 461(7), 591(0), 599(26), 603(3), 613(0), 669(511), 760(35), 762(4), 787(223), 789(6), 833(0), 833(2), 837(0), 840(32), 841(2), 845(0), 895(0), 895(17), 897(1), 898(0), 1012(0), 1012(25), 1039(5), 1039(39), 1068(0), 1070(25), 1072(0), 1074(1), 1146(0), 1146(0), 1275(0), 1275(0), 1394(0), 1399(93), 1400(0), 1408(1), 1449(4), 1450(0), 1490(10), 1491(0), 1973(1072), 2020(109), 3272(0), 3272(0), 3274(0), 3274(0), 3285(0), 3285(2), 3292(0), 3292(1), 3301(6), 3301(1)	-11(0), 5(0), 32(1), 73(0), 75(0), 77(0), 105(0), 161(9), 163(0), 187(0), 207(10), 214(0), 222(3), 230(0), 282(57), 313(2), 371(2), 417(0), 420(14), 426(1), 449(5), 562(5), 568(2), 571(0), 574(1), 644(365), 726(36), 728(8), 756(207), 757(7), 779(2), 779(0), 804(0), 807(26), 809(0), 811(0), 837(0), 839(1), 845(4), 846(1), 973(25), 973(0), 996(0), 997(33), 1030(14), 1031(0), 1033(0), 1034(0), 1099(0), 1099(0), 1222(0), 1222(0), 1329(0), 1331(1), 1340(44), 1346(1), 1390(0), 1392(7), 1417(0), 1417(0), 1852(815), 1885(150), 3163(0), 3163(0), 3165(0), 3165(1), 3176(0), 3177(4), 3182(0), 3182(3), 3191(7), 3191(0)

Table S48 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CO)_2$ **2CO-2S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
30(0), 53(0), 55(1), 58(0), 66(0), 82(0), 84(1), 114(0), 135(2), 143(9), 148(0), 155(0), 282(24), 303(0), 338(0), 341(0), 348(2), 374(0), 421(33), 430(40), 436(0), 444(0), 625(25), 625(0), 629(0), 637(0), 750(91), 755(0), 805(83), 811(0), 826(2), 827(0), 831(61), 832(0), 852(2), 859(0), 907(46), 911(8), 914(0), 919(0), 1000(0), 1002(8), 1027(19), 1029(0), 1068(0), 1069(36), 1071(0), 1075(0), 1126(1), 1129(0), 1272(0), 1272(0), 1394(27), 1398(0), 1401(0), 1403(0), 1435(0), 1439(6), 1536(40), 1549(0), 2143(1937), 2154(0), 3242(0), 3243(3), 3243(0), 3244(1), 3256(6), 3257(0), 3269(0), 3269(5), 3277(20), 3277(0)	26(0), 38(0), 52(1), 52(0), 55(0), 65(0), 79(0), 109(0), 124(2), 128(10), 137(0), 146(0), 271(14), 290(0), 318(0), 320(0), 336(2), 363(0), 417(28), 431(0), 435(17), 449(0), 592(11), 597(0), 601(0), 602(0), 716(109), 720(0), 773(82), 777(0), 794(35), 794(0), 794(2), 795(0), 815(1), 819(0), 860(9), 863(0), 865(38), 875(0), 961(0), 962(7), 985(19), 988(0), 1029(0), 1029(28), 1031(0), 1035(0), 1081(1), 1083(0), 1219(0), 1220(0), 1329(17), 1329(1), 1334(0), 1335(0), 1369(0), 1374(4), 1464(27), 1475(0), 2006(1709), 2017(0), 3135(0), 3135(3), 3135(0), 3135(0), 3147(7), 3147(0), 3160(0), 3160(7), 3168(23), 3168(0)

Table S49 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CO)_2$ **2CO-3S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
31(0), 55(0), 56(0), 60(0), 76(0), 83(0), 83(0), 109(1), 112(1), 143(8), 148(0), 162(0), 279(19), 306(0), 335(2), 336(0), 340(0), 366(1), 430(31), 434(46), 439(0), 441(1), 622(0), 629(35), 633(0), 637(0), 747(73), 753(0), 802(109), 813(2), 825(0), 826(3), 831(55), 837(0), 844(3), 855(0), 905(36), 913(0), 913(12), 922(3), 995(0), 996(7), 1023(5), 1029(16), 1064(30), 1071(0), 1071(0), 1073(4), 1126(0), 1128(1), 1272(0), 1273(0), 1388(27), 1393(2), 1395(0), 1404(0), 1435(0), 1439(3), 1552(50), 1562(3), 2144(1838), 2155(47), 3237(1), 3237(2), 3238(0), 3239(2), 3254(0), 3254(5), 3269(0), 3269(7), 3276(15), 3276(3)	27(0), 50(0), 51(0), 53(0), 68(0), 74(0), 76(0), 90(3), 102(1), 133(7), 133(0), 153(0), 265(11), 292(0), 315(0), 317(0), 321(1), 355(1), 423(34), 423(0), 445(16), 455(1), 593(0), 597(18), 602(0), 604(0), 713(89), 719(0), 771(106), 781(2), 793(0), 794(3), 795(30), 799(0), 810(3), 860(30), 862(0), 862(13), 876(3), 955(0), 957(6), 983(2), 988(17), 1023(28), 1031(0), 1031(1), 1032(3), 1082(0), 1084(2), 1220(0), 1220(0), 1322(19), 1325(3), 1326(0), 1337(0), 1367(0), 1373(2), 1480(36), 1488(3), 2008(1611), 2019(52), 3129(2), 3129(1), 3130(0), 3130(2), 3145(0), 3145(6), 3160(0), 3160(9), 3167(16), 3167(3)

Table S50 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CO)_2$ **2CO-4S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
27(1), 24(0), 38(2), 60(0), 62(0), 78(1), 93(1), 134(2), 141(5), 148(0), 175(1), 227(1), 241(1), 255(4), 281(17), 320(9), 342(7), 357(5), 405(21), 434(22), 461(17), 560(45), 585(52), 596(30), 601(22), 635(21), 742(28), 748(9), 775(106), 779(77), 809(28), 824(0), 833(2), 842(30), 843(1), 857(11), 891(0), 898(3), 905(9), 911(6), 993(5), 1003(12), 1014(10), 1043(18), 1062(17), 1068(9), 1071(8), 1088(6), 1128(1), 1146(0), 1266(0), 1274(0), 1351(3), 1387(3), 1415(63), 1422(5), 1449(41), 1462(2), 1499(1), 1531(5), 1989(515), 2146(1195), 3185(4), 3258(1), 3267(1), 3272(0), 3279(2), 3281(2), 3286(4), 3293(0), 3301(3)	20(0), 28(0), 44(1), 58(0), 62(0), 77(1), 94(1), 118(2), 136(0), 147(3), 156(1), 214(1), 229(1), 248(6), 267(7), 303(4), 333(3), 349(3), 396(17), 438(14), 451(17), 535(15), 553(26), 565(41), 573(23), 607(12), 703(37), 710(10), 741(96), 744(63), 772(28), 789(1), 796(2), 802(0), 808(21), 819(8), 842(0), 844(2), 852(5), 857(10), 953(6), 963(11), 976(9), 1001(16), 1025(13), 1029(8), 1031(5), 1045(6), 1082(1), 1099(0), 1215(0), 1222(0), 1287(4), 1323(2), 1350(49), 1360(10), 1383(27), 1391(3), 1431(0), 1457(5), 1865(416), 2010(1058), 3078(5), 3146(1), 3154(1), 3159(1), 3163(0), 3171(4), 3174(6), 3184(1), 3191(3)

Table S51 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-1S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
9(1), 11(0), 19(4), 33(7), 41(0), 43(0), 57(0), 75(2), 78(0), 113(0), 128(1), 140(8), 145(0), 148(0), 157(7), 172(0), 177(3), 184(0), 271(26), 294(0), 323(35), 336(0), 340(4), 342(0), 366(3), 381(0), 422(25), 433(0), 622(34), 624(0), 631(0), 638(0), 739(76), 746(0), 789(114), 795(0), 824(0), 826(0), 827(41), 827(0), 832(7), 835(0), 891(34), 898(10), 900(0), 904(0), 997(0), 999(8), 1024(20), 1026(0), 1033(0), 1037(0), 1066(0), 1066(29), 1069(0), 1072(0), 1123(1), 1126(0), 1134(0), 1134(0), 1136(0), 1136(0), 1270(0), 1271(0), 1393(28), 1398(0), 1400(0), 1404(0), 1435(0), 1439(4), 1448(127), 1450(0), 1485(0), 1485(23), 1487(0), 1487(23), 1532(42), 1544(0), 2266(2582), 2276(0), 3082(108), 3082 (0), 3171(0), 3171(12), 3172(0), 3172(11), 3237(0), 3237(3), 3237(1), 3237(3), 3249(7), 3249(16), 3262(0), 3262(19), 3270(32), 3270(0)	11(0), 12(0), 16(4), 31(6), 32(0), 39(0), 48(0), 50(0), 69(3), 108(0), 119(1), 124(10), 134(0), 142(0), 144(7), 152(0), 157(5), 165(0), 262(16), 285(0), 315(0), 316(0), 332(1), 336(31), 348(0), 349(0), 393(19), 405(0), 588(16), 595(0), 601(0), 601(0), 703(97), 709(0), 758(95), 762(0), 790(0), 790(0), 791(29), 794(0), 797(0), 798(5), 844(12), 846(0), 850(28), 861(0), 957(0), 959(7), 983(18), 985(0), 997(3), 1001(0), 1026(24), 1026(0), 1028(0), 1031(0), 1077(3), 1080(0), 1086(0), 1086(1), 1087(0), 1087(1), 1217(0), 1217(0), 1327(20), 1329(0), 1334(0), 1334(0), 1368(0), 1373(2), 1394(168), 1395(0), 1431(0), 1431(21), 1431(0), 1431(20), 1461(31), 1472(0), 2138(2572), 2148(0), 2968(152), 2968(0), 3046(0), 3146(19), 3148(0), 3148(16), 3127(0), 3127(3), 3127(1), 3127(5), 3138(15), 3138(9), 3052(0), 3152(23), 3160(35), 3160(0)

Table S52 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-2S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
16(0), 22(0), 32(0), 59(1), 74(1), 75(0), 85(8), 98(1), 102(0), 114(13), 131(10), 152(0), 172(0), 175(5), 183(17), 199(0), 226(60), 238(6), 246(4), 254(2), 287(86), 328(2), 382(0), 387(5), 422(12), 457(0), 491(25), 598(15), 602(12), 604(2), 611(3), 675(418), 750(22), 754(10), 775(255), 777(22), 811(0), 811(6), 840(1), 841(2), 841(17), 844(0), 878(0), 878(12), 889(4), 890(1), 1015(32), 1015(0), 1028(32), 1037(3), 1038(0), 1038(33), 1070(12), 1071(0), 1073(2), 1073(0), 1118(22), 1118(7), 1128(2), 1128(1), 1147(0), 1147(0), 1275(0), 1275(0), 1396(27), 1397(0), 1409(27), 1411(2), 1431(64), 1433(16), 1457(0), 1457(5), 1481(2), 1482(3), 1485(7), 1485(1), 1486(24), 1486(0), 1953(1437), 1993(330), 3056(119), 3057(30), 3148(22), 3148(1), 3161(1), 3161(19), 3267(1), 3267(0), 3271(0), 3271(0), 3282(0), 3282(8), 3288(1), 3288(3), 3298(8), 3298(1)	22(0), 28(0), 32(0), 56(2), 72(1), 74(0), 84(4), 89(1), 91(0), 112(10), 131(9), 143(0), 158(14), 160(0), 164(4), 185(0), 217(14), 219(2), 237(34), 243(6), 282(56), 315(1), 368(8), 377(0), 402(5), 435(0), 487(23), 563(5), 568(2), 569(7), 581(4), 655(323), 710(18), 714(12), 741(226), 742(16), 767(15), 767(0), 806(0), 807(1), 808(10), 810(0), 829(0), 829(11), 838(2), 839(1), 974(41), 974(0), 976(10), 983(1), 996(0), 997(32), 1031(8), 1032(0), 1033(0), 1033(1), 1072(6), 1072(13), 1079(0), 1079(2), 1100(0), 1100(0), 1221(0), 1221(0), 1333(17), 1336(0), 1344(17), 1346(1), 1374(67), 1376(20), 1394(0), 1395(5), 1416(3), 1416(0), 1428(7), 1428(0), 1431(20), 1431(2), 1842(1068), 1871(285), 2946(131), 2946(37), 3031(27), 3031(1), 3043(2), 3043(23), 3157(1), 3157(0), 3161(0), 3161(0), 3172(0), 3172(13), 3178(2), 3178(7), 3188(10), 3188(1)

Table S53 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-3S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
14(0), 14(0), 20(4), 34(7), 42(0), 42(1), 74(0), 75(2), 88(0), 104(1), 114(1), 139(8), 145(0), 153(4), 167(3), 173(1), 175(4), 178(0), 263(22), 298(0), 325(23), 337(0), 341(13), 347(1), 362(3), 383(1), 424(28), 429(0), 622(0), 625(47), 635(0), 735(62), 742(0), 786(130), 799(3), 821(0), 825(0), 828(35), 829(9), 832(0), 834(0), 891(30), 899(0), 900(15), 908(2), 993(0), 995(8), 1020(7), 1025(16), 1035(1), 1038(0), 1061(23), 1069(0), 1069(0), 1069(4), 1122(1), 1125(1), 1135(0), 1135(0), 1135(0), 1135(0), 1270(0), 1270(0), 1386(30), 1394(0), 1395(0), 1402(0), 1435(0), 1439(2), 1448(119), 1449(3), 1485(0), 1485(23), 1486(3), 1486(20), 1550(56), 1559(1), 2269(2422), 2279(80), 3082(99), 3082 (5), 3171(2), 3171(9), 3172(2), 3172(10), 3230(4), 3230(5), 3230 (0), 3231(5), 3244(0), 3244(0), 3244(22), 3262(4), 3262(25), 3269(22), 3269(0)	18(0), 18(0), 19(3), 33(6), 38(0), 40(1), 62(0), 69(2), 79(0), 84(3), 107(0), 127(9), 132(0), 142(5), 153(5), 155(0), 160(1), 160(2), 252(13), 287(0), 313(0), 314(0), 327(2), 336(20), 354(2), 357(10), 396(21), 398(0), 593(25), 593(0), 599(0), 605(0), 701(81), 707(0), 755(114), 767(3), 788(0), 791(19), 793(0), 794(0), 797(8), 798(0), 847(0), 848(27), 848(16), 863(3), 953(0), 955(7), 980(3), 984(17), 1000(4), 1004(0), 1020(21), 1028(2), 1028(0), 1029(0), 1078(3), 1080(2), 1087(0), 1087(1), 1087(1), 1088(0), 1217(0), 1217(0), 1320(22), 1325(0), 1327(0), 1335(0), 1366(0), 1372(1), 1394(154), 1395(5), 1431(0), 1431(21), 1432(4), 1432(18), 1479(45), 1487(1), 2142(2387), 2152(100), 2968(137), 2968(9), 3047(1), 3047(16), 3047(3), 3047(15), 3120(5), 3120(4), 3120(0), 3121(6), 3134(0), 3134(22), 3052(5), 3152(29), 3159(24), 3159(0)

Table S54 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CNCH_3)_2$ **2CNCH$_3$-4S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
20(0), 26(0), 30(0), 59(2), 69(0), 83(1), 90(2), 106(1), 108(1), 119(1), 129(33), 148(4), 168(8), 174(2), 180(16), 200(2), 220(23), 240(8), 244(15), 258(3), 284(73), 332(6), 376(9), 406(43), 411(8), 458(2), 488(46), 597(12), 601(7), 604(3), 613(3), 679(388), 751(31), 757(17), 779(189), 783(83), 800(0), 818(2), 839(0), 840(3), 841(13), 844(4), 873(1), 883(2), 885(4), 891(4), 1014(16), 1015(16), 1027(16), 1036(17), 1037(28), 1039(21), 1070(12), 1071(1), 1072(1), 1072(0), 1119(24), 1119(8), 1128(1), 1128(0), 1147(0), 1147(0), 1274(0), 1274(0), 1395(15), 1397(3), 1410(27), 1413(8), 1431(66), 1434(15), 1456(4), 1460(2), 1477(1), 1484(3), 1485(4), 1485(2), 1486(16), 1486(10), 1952(1404), 1993(347), 3056(95), 3057(58), 3148(13), 3148(9), 3061(7), 3161(13), 3267(0), 3268(0), 3270(0), 3273(1), 3280(5), 3285(3), 3286(3), 3290(2), 3296(5), 3300(4)	15(0), 23(0), 31(0), 56(2), 68(1), 77(1), 84(1), 97(0), 99(1), 115(1), 130(17), 141(6), 151(6), 164(4), 165(13), 187(1), 202(9), 230(4), 236(9), 240(20), 281(47), 319(4), 364(0), 389(28), 403(8), 438(2), 482(47), 563(5), 567(2), 570(4), 583(5), 667(297), 713(28), 717(17), 747(173), 750(70), 757(1), 772(2), 804(0), 807(2), 807(10), 810(2), 827(1), 833(1), 835(3), 839(3), 973(27), 974(12), 976(2), 983(18), 994(14), 997(18), 1031(7), 1031(2), 1032(0), 1033(0), 1072(8), 1072(14), 1078(0), 1078(1), 1100(0), 1100(0), 1221(0), 1221(0), 1332(10), 1336(1), 1344(16), 1347(5), 1374(69), 1377(20), 1393(3), 1398(2), 1412(1), 1418(1), 1428(2), 1428(6), 1431(14), 1431(8), 1841(1036), 1872(310), 2944(101), 2945(71), 3031(17), 3031(11), 3043(9), 3043(16), 3157(0), 3158(0), 3160(0), 3163(1), 3171(8), 3175(6), 3175(5), 3180(3), 3185(6), 3190(5)

Table S55 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CS)_2$ **2CS-1S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
-4(0), -3(0), 33(0), 66(0), 76(0), 81(0), 102(1), 147(1), 177(1), 177(0), 206(20), 214(0), 245(6), 257(0), 288(72), 316(4), 323(0), 377(6), 378(19), 413(2), 426(0), 596(2), 599(9), 600(0), 601(1), 634(215), 769(85), 773(13), 793(196), 795(6), 818(0), 819(5), 839(0), 841(11), 841(4), 843(0), 888(0), 889(1), 896(5), 897(1), 1018(0), 1018(24), 1036(0), 1037(32), 1070(0), 1071(4), 1071(1), 1072(0), 1148(0), 1148(0), 1233(954), 1274(0), 1294(175), 1396(9), 1396(0), 1406(7), 1409(6), 1459(0), 1461(11), 1478(1), 1479(1), 3273(0), 3274(0), 3276(0), 3276(0), 3288(0), 3288(1), 3291(0), 3291(1), 3302(4), 3302(1)	13(0), 13(0), 34(1), 65(0), 73(0), 80(0), 101(1), 140(0), 168(0), 169(0), 180(17), 190(0), 219(5), 229(0), 278(47), 301(3), 308(0), 358(11), 363(5), 400(1), 419(0), 562(1), 566(1), 568(5), 569(0), 608(167), 728(70), 732(13), 758(187), 759(4), 773(0), 773(7), 806(0), 808(7), 809(2), 810(0), 838(0), 839(0), 844(4), 845(1), 979(0), 979(22), 995(0), 995(30), 1032(0), 1032(2), 1032(1), 1034(0), 1101(0), 1101(0), 1173(713), 1222(0), 1222(0), 1225(137), 1334(6), 1335(0), 1341(4), 1344(3), 1397(0), 1398(9), 1413(1), 1413(1), 3164(0), 3164(0), 3166(0), 3166(0), 3178(0), 3178(4), 3181(0), 3181(3), 3192(6), 3192(1)

Table S56 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CS)_2$ **2CS-2S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
17(1), 28(0), 40(1), 47(1), 54(1), 75(2), 89(1), 120(9), 138(2), 153(1), 163(0), 177(3), 224(1), 234(2), 281(17), 297(8), 311(8), 334(1), 342(19), 382(4), 415(3), 555(65), 584(32), 594(5), 599(42), 626(22), 747(10), 750(26), 771(104), 779(67), 799(62), 829(0), 832(5), 836(3), 841(25), 851(9), 887(1), 895(3), 900(15), 908(3), 998(3), 1007(10), 1016(9), 1041(15), 1066(18), 1069(10), 1070(5), 1085(5), 1128(1), 1147(0), 1232(414), 1266(0), 1275(0), 1357(2), 1373(944), 1387(4), 1415(55), 1423(9), 1448(23), 1457(2), 1498(1), 1516(6), 3197(3), 3263(1), 3265(1), 3272(0), 3274(0), 3280(3), 3285(1), 3292(3), 3292(1), 3300(3)	20(0), 26(0), 36(1), 42(0), 53(1), 73(2), 89(0), 117(2), 135(0), 143(4), 148(0), 165(3), 211(1), 239(3), 267(6), 274(7), 306(3), 321(1), 328(20), 370(1), 401(6), 519(61), 549(12), 564(20), 570(6), 603(12), 709(39), 715(17), 741(61), 743(99), 765(30), 787(6), 791(1), 803(0), 807(19), 814(7), 837(1), 838(3), 845(7), 860(7), 949(8), 967(9), 974(9), 999(15), 1026(12), 1030(4), 1031(5), 1042(7), 1079(1), 1100(0), 1177(336), 1212(0), 1221(0), 1287(2), 1299(749), 1326(5), 1348(30), 1360(13), 1379(14), 1390(7), 1430(2), 1452(6), 3079(4), 3147(2), 3156(1), 3157(1), 3163(0), 3167(2), 3171(4), 3175(7), 3183(1), 3191(4)

Table S57 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CS)_2$ **2CS-3S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
16(0), 36(0), 36(0), 46(0), 63(1), 78(1), 90(0), 110(0), 133(0), 134(2), 140(15), 149(0), 268(15), 299(0), 304(7), 321(0), 336(0), 344(0), 370(12), 382(0), 384(10), 398(0), 624(17), 628(0), 631(0), 638(0), 753(96), 758(0), 803(91), 809(0), 825(7), 827(0), 829(61), 830(0), 845(1), 854(0), 898(41), 911(0), 911(6), 914(0), 1001(0), 1002(7), 1026(20), 1028(0), 1069(29), 1069(1), 1072(0), 1075(0), 1124(1), 1127(0), 1272(0), 1273(0), 1354(1846), 1372(0), 1392(17), 1398(0), 1398(19), 1404(0), 1434(0), 1439(87), 1533(29), 1546(0), 3246(0), 3246(2), 3247(0), 3247(0), 3258(0), 3258(0), 3268(0), 3268(6), 3277(22), 3277(0)	12(0), 32(0), 33(0), 41(0), 57(0), 63(0), 72(1), 104(0), 116(0), 122(2), 125(14), 144(0), 261(10), 286(0), 291(5), 309(0), 317(0), 324(0), 369(2), 372(6), 378(0), 384(0), 592(7), 599(0), 602(0), 603(0), 719(114), 724(0), 770(87), 775(0), 791(0), 792(34), 793(5), 795(0), 808(1), 813(0), 855(33), 860(7), 862(0), 866(0), 962(0), 963(6), 984(19), 986(0), 1029(21), 1029(1), 1032(0), 1035(0), 1079(1), 1082(0), 1219(0), 1220(0), 1294(1391), 1310(0), 1327(9), 1330(34), 1332(0), 1335(0), 1368(0), 1374(59), 1460(17), 1472(0), 3137(0), 3137(3), 3138(0), 3138(0), 3148(6), 3149(0), 3159(0), 3159(7), 3167(24), 3168(0)

Table S58 Theoretical harmonic vibrational frequencies (in cm^{-1}) and IR intensities (in km/mol) of $Cp_2Pd_2(CS)_2$ **2CS-4S** by MPW1PW91 and BP86 methods

MPW1PW91	BP86
19(0), 37(1), 40(0), 44(0), 74(1), 75(0), 91(0), 108(1), 119(1), 132(0), 140(14), 161(0), 274(17), 279(3), 306(0), 312(4), 332(0), 341(0), 380(8), 387(1), 388(12), 390(0), 623(0), 629(24), 634(0), 636(0), 751(79), 757(1), 798(120), 811(2), 825(0), 826(13), 828(41), 835(1), 836(2), 850(0), 895(29), 914(0), 914(3), 914(13), 996(0), 997(5), 1023(3), 1029(17), 1062(26), 1070(4), 1071(0), 1071(3), 1124(1), 1127(2), 1273(0), 1273(0), 1359(1697), 1378(84), 1385(18), 1392(5), 1395(0), 1400(0), 1431(0), 1436(87), 1553(41), 1562(2), 3240(1), 3240(2), 3241(0), 3241(1), 3255(0), 3255(4), 3267(6), 3267(0), 3276(16), 3276(3)	18(0), 36(0), 38(0), 41(0), 69(1), 73(0), 78(0), 93(2), 113(1), 119(0), 130(11), 154(0), 261(10), 268(3), 293(0), 301(3), 310(2), 317(0), 371(0), 376(8), 379(0), 384(0), 594(0), 595(11), 600(0), 604(0), 718(95), 723(2), 764(112), 778(3), 790(15), 793(0), 793(10), 795(1), 802(3), 811(0), 848(22), 863(0), 863(15), 866(3), 957(0), 958(4), 983(1), 988(17), 1022(22), 1030(6), 1030(2), 1031(0), 1080(1), 1082(2), 1220(0), 1220(0), 1299(1233), 1315(88), 1319(11), 1324(19), 1325(0), 1333(0), 1364(0), 1370(62), 1480(27), 1487(3), 3129(1), 3129(2), 3131(0), 3131(2), 3146(0), 3146(4), 3157(0), 3158(8), 3167(17), 3167(4)

Complete Gaussian 09 reference (Reference 10)

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