Electronic Supporting Information

Theoretical study on the leaching of palladium in a CO atmosphere[†]

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S1. The most stable CO adsorption site on investigated models at low coverage

At low coverage (1/12 ML), all possible CO adsorption sites around the Pd atom to be leached out were investigated and Figure S1 just gives the most table ones for further inspection as listed in Table 1 of the main text.
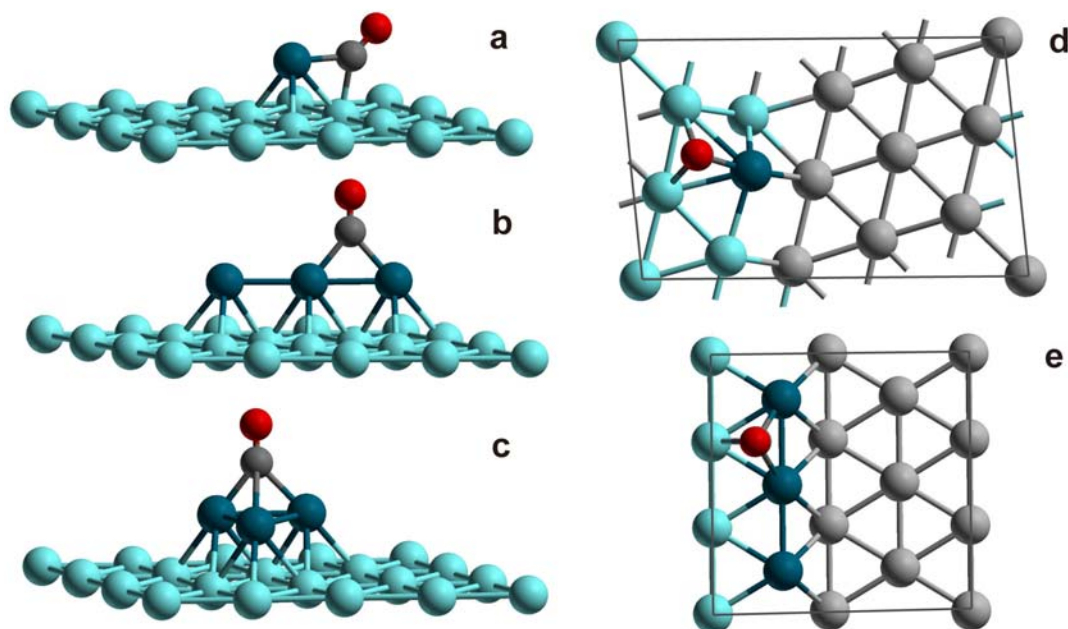
Figure S1. The most stable site for one CO adsorption on investigated models: (a) Pd_1, (b) Pd_3 line, (c) Pd_3 triangle, (d) Pd(865) and (e) Pd(221). Dark blue-colored atoms represent additional atoms on Pd(111), kink atoms of Pd(865) and step atoms of Pd(221). For Pd(865) and Pd(221), upper layer atoms are in light blue and terrace atoms are in gray.

Table S1 Adsorption energy of CO at the top site of various models (kJ mol^{-1})

Model	E_{ad}(CO)	Model	E_{ad}(CO)
Pd_1	154	Pd(865)	149
Pd_3 line	156	Pd(221)	148
Pd_3 triangle	160	Pd(111)	135

S2. Selected high coverage models of Pd_1, Pd_3 line and Pd(865)

Figure S2 gives the visual pictures of high coverage models, corresponding to the models listed in Table 2 of the main text. Taking Pd_1 models for example, T+B (1), T+T and T+B (2) are 9COs-adsorbed cases with two CO directly interacted with the Pd atom to be leached out at top (T) or bridge (B) site. While T+T+B (1) and T+T+B (2) are 10COs-adsorbed cases with three CO directly interacted with the Pd atom to be leached out at T or B site. For Pd_3 line and Pd(865), they also consist of 9COs- and 10COs-adsorbed models and the adsorption rules are the same as Pd_1. H stands for hollow site.

Pd₁ high coverage models:
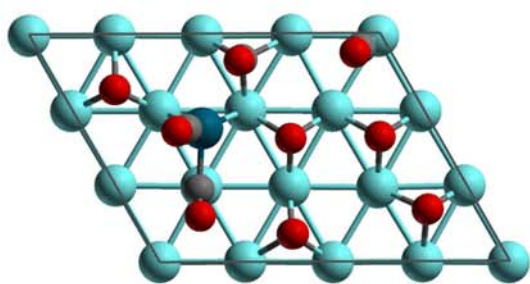
T+B (1)
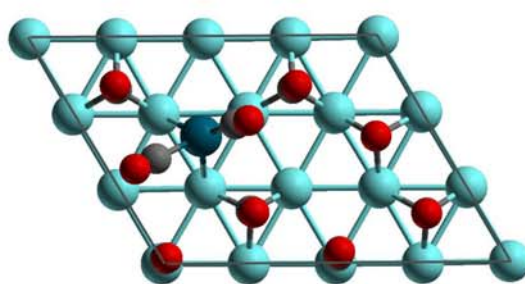
T+T

T+B (2)

T+T+B (1)

T+T+B (2)

Pd₃ line high coverage models:

B+B

T+B

T+B+B

T+T+B

Pd(865) high coverage models:
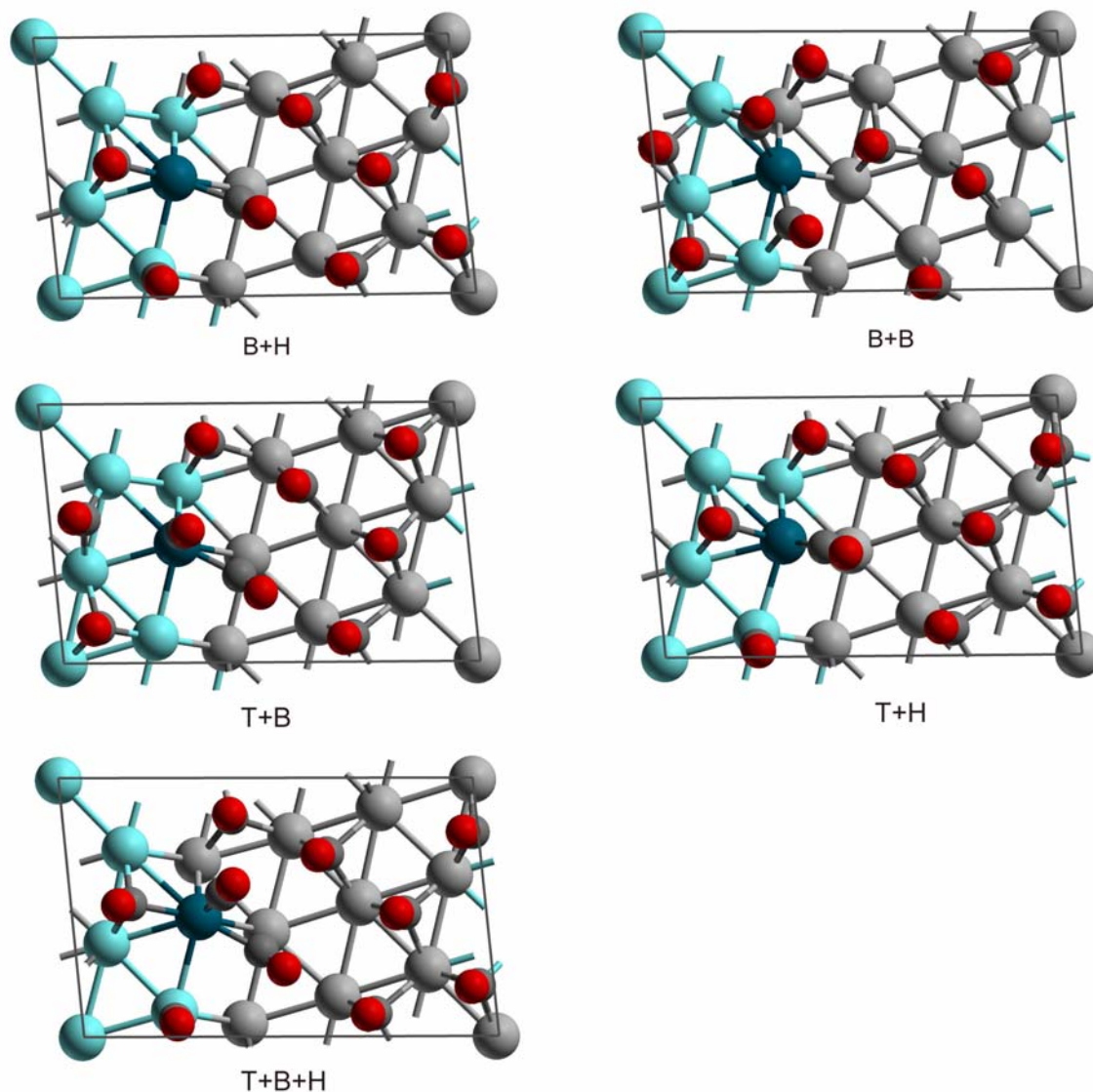
Figure S2. High CO coverage models of Pd_1, Pd_3 line and Pd(865). Different colored atoms are illustrated in the notes of Figure S1.
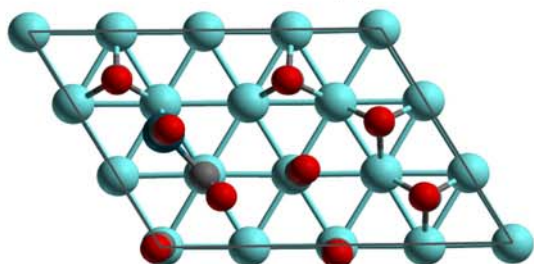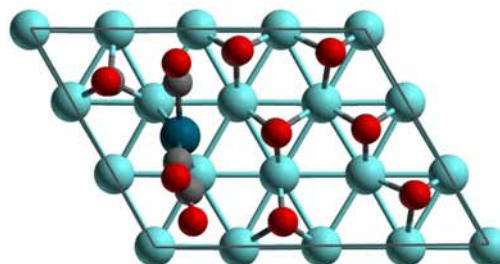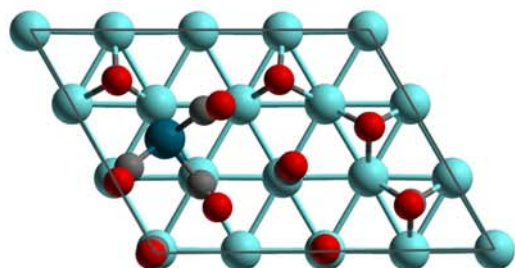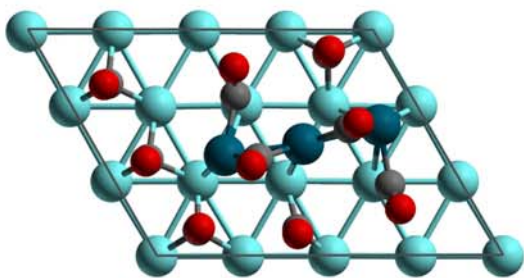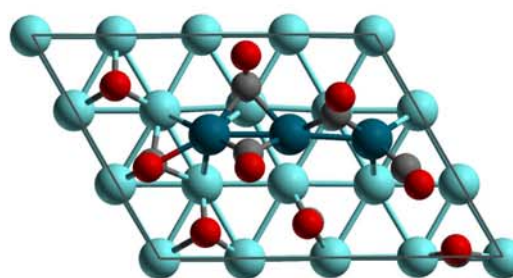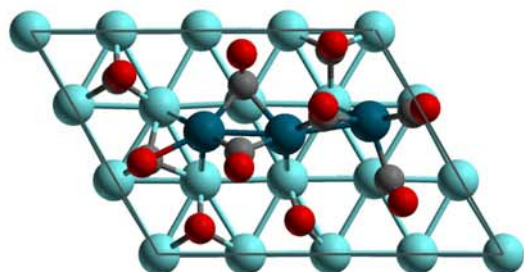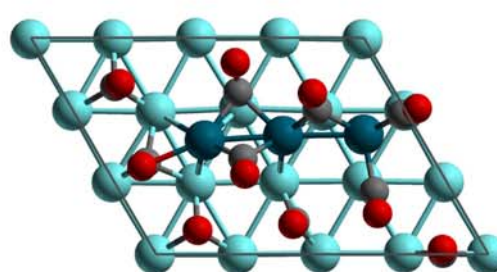
S3. Cartesian Coordinates

Here we list the Cartesian coordinates (Å) of the optimized structures listed in Table 1 (depicted in Figure S1) and Table 2 (depicted in Figure S2) of the main text. For each model, the two bottom layers are kept fixed during optimization. Thus, the coordinates of the Pd atoms in the two bottom layers are listed first. In the subsequent tables only the optimized coordinates of the Pd atoms and adsorbates are listed.

Two bottom layers of Pd surfaces

Two bottom layers of Pd(111)

Pd	0.00000	1.61670	2.28630	Pd	0.00000	0.00000	0.00000
Pd	2.80010	1.61670	2.28630	Pd	2.80010	0.00000	0.00000
Pd	5.60030	1.61670	2.28630	Pd	5.60030	0.00000	0.00000
Pd	8.40040	1.61670	2.28630	Pd	8.40040	0.00000	0.00000
Pd	-1.40010	4.04170	2.28630	Pd	9.80050	2.42500	0.00000
Pd	1.40010	4.04170	2.28630	Pd	1.40010	2.42500	0.00000
Pd	4.20020	4.04170	2.28630	Pd	4.20020	2.42500	0.00000
Pd	7.00040	4.04170	2.28630	Pd	7.00040	2.42500	0.00000
Pd	-2.80010	6.46670	2.28630	Pd	-2.80010	4.85000	0.00000
Pd	0.00000	6.46670	2.28630	Pd	0.00000	4.85000	0.00000
Pd	2.80010	6.46670	2.28630	Pd	2.80010	4.85000	0.00000
Pd	5.60030	6.46670	2.28630	Pd	5.60030	4.85000	0.00000

Two bottom layers of Pd(221)

Pd	1.40010	4.20020	2.64000	Pd	0.00000	5.60030	0.66000
Pd	1.40010	0.46670	3.96000	Pd	0.00000	1.86680	1.98000
Pd	0.00000	6.53370	3.30000	Pd	1.40010	3.26680	0.00000
Pd	0.00000	2.80010	4.62000	Pd	1.40010	7.93370	1.32000
Pd	4.20020	4.20020	2.64000	Pd	2.80010	5.60030	0.66000
Pd	4.20020	0.46670	3.96000	Pd	2.80010	1.86680	1.98000
Pd	2.80010	6.53370	3.30000	Pd	4.20020	3.26680	0.00000
Pd	2.80010	2.80010	4.62000	Pd	4.20020	7.93370	1.32000
Pd	7.00040	4.20020	2.64000	Pd	5.60030	5.60030	0.66000
Pd	7.00040	0.46670	3.96000	Pd	5.60030	1.86680	1.98000
Pd	5.60030	6.53370	3.30000	Pd	7.00040	3.26680	0.00000
Pd	5.60030	2.80010	4.62000	Pd	7.00040	7.93370	1.32000

Two bottom layers of Pd(865)

Pd	6.31989	1.97168	3.36484	Pd	6.31989	11.24856	0.53129
Pd	1.02812	3.77026	3.71903	Pd	2.61565	0.31509	0.70839
Pd	3.14483	10.20728	2.65645	Pd	6.84907	3.91225	1.41677

Pd	3.67400	2.87097	3.54193	Pd	1.55729	5.71083	1.77097
Pd	5.79071	9.30799	2.47935	Pd	4.73236	2.11367	1.06258
Pd	1.55729	1.07239	3.18774	Pd	6.84907	8.55069	0.00000
Pd	3.67400	7.50941	2.12516	Pd	1.55729	10.34927	0.35419
Pd	5.79071	4.66955	3.89612	Pd	7.37824	1.21438	0.88548
Pd	7.90742	11.10657	2.83355	Pd	2.08647	3.01296	1.23968
Pd	4.20318	0.17310	3.01064	Pd	4.20318	9.44998	0.17710
Pd	1.02812	8.40870	2.30226	Pd	6.31989	6.61012	1.94806
Pd	3.14482	5.56884	4.07322	Pd	6.31989	11.24856	0.53129

Cartesian Coordinates of low coverage models (Table 1 of the text):

Pd$_1$_ Bridge

C	4.13926	2.52368	8.97297	Pd	5.68440	4.84648	6.80345
O	4.09361	1.82513	9.92608	Pd	1.38844	0.79324	4.54982
Pd	4.18461	4.49071	8.94809	Pd	4.19351	0.81201	4.59518
Pd	7.00388	7.25981	6.84681	Pd	7.00235	0.78537	4.56314
Pd	-1.42252	7.24105	6.84492	Pd	9.79150	0.78746	4.55901
Pd	1.37761	7.25078	6.84893	Pd	-0.00642	3.22202	4.55056
Pd	4.19245	7.21366	6.88277	Pd	2.80420	3.20242	4.57477
Pd	9.78405	2.37933	6.84513	Pd	5.58409	3.19609	4.58074
Pd	1.35683	2.39613	6.84287	Pd	8.39227	3.21619	4.55142
Pd	4.18594	2.38986	7.01468	Pd	-1.40642	5.65309	4.54705
Pd	7.02034	2.38031	6.85034	Pd	1.39028	5.64891	4.54736
Pd	8.41737	4.81152	6.84905	Pd	4.19533	5.63872	4.55743
Pd	-0.04458	4.82466	6.84739	Pd	6.99599	5.63824	4.55140
Pd	2.69651	4.84415	6.79602				

Pd$_3$ line_ Bridge

C	5.55703	3.72782	10.37972	Pd	2.80829	4.89690	6.78380
O	5.58842	3.49983	11.53632	Pd	5.58645	4.89745	6.78411
Pd	1.49139	3.95252	8.87641	Pd	1.39879	0.80431	4.57425
Pd	4.16210	4.04522	9.00714	Pd	4.19287	0.81331	4.57652
Pd	6.90263	4.09456	8.96834	Pd	6.99540	0.80830	4.56956
Pd	7.00387	7.25130	6.88202	Pd	9.80315	0.80382	4.57201
Pd	-1.40749	7.23538	6.87476	Pd	-0.00573	3.22644	4.56187
Pd	1.38552	7.24381	6.87000	Pd	2.79403	3.22847	4.55524
Pd	8.40580	0.02075	6.87162	Pd	5.59634	3.22632	4.55155
Pd	-1.39569	2.42249	6.88383	Pd	8.40026	3.22466	4.57092
Pd	1.39959	2.33507	6.84028	Pd	-1.39528	5.65414	4.56428
Pd	4.19047	2.37354	6.87155	Pd	1.37877	5.66624	4.54159
Pd	6.98735	2.37445	6.86216	Pd	4.19232	5.66574	4.54854

| Pd | -2.77736 | 4.83619 | 6.87016 | Pd | 7.01092 | 5.65792 | 4.55514 |
| Pd | -0.02943 | 4.84936 | 6.86082 | | | | |

Pd₃ triangle_ Hollow

C	2.81456	3.23402	10.25906	Pd	2.80359	4.89653	6.80667
O	2.81617	3.22771	11.45515	Pd	5.65191	4.87733	6.86052
Pd	1.42053	4.04629	8.98534	Pd	1.39927	0.80430	4.56018
Pd	4.20702	4.04235	8.98240	Pd	4.20034	0.79915	4.56643
Pd	2.80986	1.62901	8.97775	Pd	6.99608	0.80180	4.57542
Pd	7.00010	7.26709	6.87635	Pd	9.79766	0.80387	4.56778
Pd	-1.41322	7.22446	6.85837	Pd	-0.00988	3.22869	4.56018
Pd	1.38588	7.26071	6.89321	Pd	2.79853	3.23037	4.54287
Pd	8.40754	0.00529	6.87827	Pd	5.60698	3.23563	4.56032
Pd	9.77474	2.41530	6.87366	Pd	8.39569	3.22664	4.56418
Pd	1.34754	2.39611	6.80904	Pd	-1.40975	5.64914	4.54718
Pd	4.25021	2.40123	6.80502	Pd	1.39042	5.65713	4.56872
Pd	7.01083	2.42197	6.87613	Pd	4.20468	5.66043	4.56280
Pd	8.39383	4.83915	6.86738	Pd	7.01011	5.66575	4.55633
Pd	-0.05676	4.84847	6.86384				

Pd(865)_ Hollow

C	3.65790	1.72447	9.27170	Pd	8.44399	11.67805	7.56556
O	3.66078	1.55672	10.45274	Pd	3.14957	0.93277	5.47268
Pd	4.25100	3.41319	8.24520	Pd	5.26396	7.35695	4.43695
Pd	2.09235	6.34902	6.59785	Pd	7.37359	4.56673	6.28717
Pd	6.30072	9.89987	7.25122	Pd	5.78885	0.03273	5.29736
Pd	4.73695	5.44723	6.44442	Pd	0.52707	1.84230	5.62452
Pd	6.88470	2.52147	8.01703	Pd	7.90685	6.45232	4.28000
Pd	3.66593	10.75074	7.40351	Pd	2.60742	8.25422	4.59594
Pd	4.73710	0.70638	7.82142	Pd	2.57877	3.68060	6.06193
Pd	6.84818	7.23187	6.75841	Pd	4.73325	10.05307	4.92682
Pd	1.53769	9.01583	7.08377	Pd	5.26379	2.74707	5.79448
Pd	2.06474	1.63055	7.96286	Pd	7.37266	9.16049	4.77347
Pd	4.19475	8.11102	6.90835	Pd	2.08973	10.95275	5.10081

Pd(221)_ Hollow

C	4.21205	3.55863	10.90564	Pd	5.63388	4.60285	9.84665
O	4.22704	3.32382	12.07559	Pd	8.40255	7.46192	5.91991
Pd	2.77436	4.59635	9.85478	Pd	8.40232	3.74382	7.18317
Pd	8.40259	8.37534	8.56608	Pd	1.40383	5.15077	5.25913
Pd	1.40403	6.10517	7.96074	Pd	1.40024	1.38594	6.56797

Pd	1.37952	2.26043	9.17967	Pd	2.80202	7.46422	5.94835
Pd	0.00101	4.56416	9.73507	Pd	2.79970	3.75842	7.23243
Pd	2.79676	0.00186	8.59656	Pd	4.19949	5.14816	5.27245
Pd	4.19971	6.12470	7.98177	Pd	4.19906	1.40840	6.60845
Pd	4.20182	2.26093	9.29218	Pd	5.59777	7.46405	5.94834
Pd	5.60279	0.00152	8.59519	Pd	5.59996	3.75793	7.22851
Pd	6.99893	6.10581	7.95750	Pd	6.99747	5.15158	5.25708
Pd	7.02205	2.26133	9.17877	Pd	6.99983	1.38625	6.56790

Pd(111)_ Hollow

C	4.20198	4.03079	8.21125	Pd	5.61704	4.85148	6.93773
O	4.20367	4.02803	9.40228	Pd	1.39484	0.79702	4.55003
Pd	6.99789	7.26682	6.84794	Pd	4.20237	0.81566	4.57384
Pd	-1.40575	7.26146	6.84804	Pd	7.00470	0.80622	4.54768
Pd	1.40650	7.27279	6.84815	Pd	9.79970	0.80421	4.55208
Pd	4.20416	7.29742	6.84528	Pd	0.00113	3.23254	4.54774
Pd	9.80631	2.42799	6.83878	Pd	2.80100	3.22881	4.57885
Pd	1.36900	2.40310	6.83963	Pd	5.59678	3.22930	4.57782
Pd	4.19672	2.39683	6.93690	Pd	8.40325	3.23331	4.54811
Pd	7.02995	2.40891	6.83966	Pd	-1.39689	5.66066	4.54965
Pd	8.40057	4.83989	6.84356	Pd	1.41447	5.65271	4.57283
Pd	0.00081	4.84893	6.84379	Pd	4.19898	5.65188	4.57873
Pd	2.78472	4.84975	6.93973	Pd	6.98490	5.64553	4.57559

Cartesian Coordinates of high coverage models (Table 2 of the text):

Pd$_1$_T+B (1)

C	2.30495	1.83968	11.26856	Pd	8.46653	0.01442	6.94333
C	-1.49404	7.18519	9.06385	Pd	-1.37992	2.45201	6.88221
C	7.89565	4.46414	8.70422	Pd	1.37660	2.41952	6.92154
C	0.02149	3.10788	8.28924	Pd	4.20152	2.41871	6.98647
C	8.50701	1.61252	8.28505	Pd	7.02449	2.39481	6.95456
C	5.81686	6.52985	8.26601	Pd	-2.79749	4.84618	6.90902
C	1.48650	5.74124	8.32040	Pd	0.03044	4.85001	7.02311
C	4.08121	4.08356	8.25001	Pd	2.78716	4.87228	6.86997
C	5.63528	1.54629	8.28534	Pd	5.58588	4.85422	6.98715
O	1.98768	1.76918	12.36765	Pd	1.41174	0.79761	4.59617
O	-1.45948	6.31446	9.85627	Pd	4.18556	0.80542	4.60184
O	7.70650	4.31050	9.83043	Pd	7.00696	0.79894	4.56859
O	-0.01356	3.10754	9.47466	Pd	9.81298	0.81423	4.53970
O	8.51320	1.59933	9.46331	Pd	0.00220	3.24408	4.57142
O	5.85510	6.55255	9.44732	Pd	2.80875	3.22115	4.58584

O	1.53621	5.74807	9.49796	Pd	5.60092	3.22463	4.60034
O	3.98866	4.03871	9.44638	Pd	8.39029	3.22716	4.56760
O	5.65212	1.54282	9.47040	Pd	-1.41496	5.66111	4.67723
Pd	2.79943	1.86522	9.35688	Pd	1.38802	5.65818	4.56896
Pd	0.04282	-0.01093	6.84686	Pd	4.20999	5.66510	4.56669
Pd	2.78404	0.00497	7.06881	Pd	6.99160	5.63567	4.56389
Pd	1.39551	7.26426	6.89914				

Pd_1_T+T

C	3.82390	2.07008	10.83601	Pd	8.44224	0.00564	6.96978
C	1.26260	0.97220	10.30522	Pd	-1.38869	2.43168	6.94041
C	-2.66414	5.01895	8.77100	Pd	1.37811	2.40782	6.96934
C	0.11096	6.55303	8.22299	Pd	4.23689	2.43748	7.06493
C	8.34963	1.64723	8.30110	Pd	7.01692	2.41649	6.89432
C	5.67640	3.21116	8.29605	Pd	-2.76559	4.87336	6.88612
C	0.02239	3.24235	8.27503	Pd	0.02858	4.84730	6.89702
C	5.76258	6.44191	8.25131	Pd	2.82577	4.83350	6.94190
C	2.89807	5.08347	8.81657	Pd	5.62785	4.83800	6.89662
O	0.58606	0.64039	11.17227	Pd	1.42354	0.80908	4.61589
O	4.24414	2.17541	11.89915	Pd	4.20649	0.82838	4.58123
O	-2.60283	5.04923	9.91990	Pd	7.02137	0.79876	4.57840
O	0.20256	6.49384	9.40922	Pd	9.81968	0.81024	4.56522
O	8.34895	1.65741	9.48129	Pd	0.02116	3.22044	4.58067
O	5.80253	3.31443	9.47082	Pd	2.82063	3.24293	4.64474
O	-0.03237	3.33551	9.45812	Pd	5.60436	3.22296	4.59221
O	5.76236	6.41734	9.43557	Pd	8.41519	3.24519	4.57447
O	2.94924	5.20889	9.96071	Pd	-1.38317	5.66925	4.56784
Pd	2.72037	1.70145	9.22872	Pd	1.42154	5.64470	4.55510
Pd	-4.15411	7.26642	6.91343	Pd	4.21021	5.66625	4.58563
Pd	2.84481	0.02032	6.96124	Pd	7.01999	5.65228	4.55815
Pd	1.42624	7.27151	6.85691				

$Pd_1\_T+B\ (2)$

C	1.71284	1.41867	11.33326	Pd	8.43926	0.03460	6.96789
C	-1.33328	7.21678	9.08179	Pd	-1.39416	2.45984	6.85798
C	8.28840	4.75288	8.80063	Pd	1.39537	2.44113	6.83845
C	5.91747	0.04215	8.78464	Pd	4.20222	2.44900	6.93506
C	8.44749	1.71611	8.26919	Pd	6.99906	2.44441	6.91704
C	5.54751	3.16294	8.28767	Pd	-2.78445	4.89080	6.91368
C	0.05645	3.26766	8.13071	Pd	-0.00125	4.87108	6.90279
C	5.71566	6.45468	8.28320	Pd	2.79907	4.86694	6.91994
C	2.88642	4.60746	8.79200	Pd	5.60427	4.84913	6.93968
O	1.89425	1.45382	12.46517	Pd	1.40486	0.79663	4.60034

O	-0.76425	6.49570	9.82561	Pd	4.19867	0.79334	4.62957
O	8.18357	4.64384	9.94068	Pd	7.00425	0.80601	4.58086
O	6.11079	0.11727	9.91757	Pd	9.80689	0.80558	4.55401
O	8.48535	1.74220	9.44976	Pd	-0.00385	3.24739	4.53847
O	5.54579	3.14610	9.47239	Pd	2.81176	3.23530	4.56463
O	0.10383	3.19535	9.34484	Pd	5.60144	3.23587	4.57725
O	5.70257	6.44610	9.46918	Pd	8.39260	3.25271	4.55495
O	2.93425	4.51364	9.94018	Pd	-1.40978	5.68385	4.62344
Pd	1.58670	1.40092	9.36997	Pd	1.40806	5.66177	4.59279
Pd	0.02363	0.01413	6.95931	Pd	4.19629	5.66927	4.59658
Pd	2.80479	0.04378	7.08735	Pd	7.00336	5.66248	4.57831
Pd	5.59546	0.01836	6.92018				

Pd_1_T+T+B (1)

C	2.16329	3.18993	10.71056	Pd	5.61971	0.01319	6.90797
C	2.15807	0.53470	11.51829	Pd	8.49679	0.02502	6.96165
C	-1.62239	6.79886	8.96051	Pd	-1.37181	2.44982	6.86735
C	7.29508	4.15909	8.28560	Pd	1.40638	2.42013	7.11474
C	-0.07944	3.17040	8.30876	Pd	4.20162	2.45283	7.05010
C	8.49696	1.60434	8.30694	Pd	7.02406	2.42858	6.99883
C	5.90596	6.65350	8.27870	Pd	-2.75231	4.86332	6.80659
C	1.51288	5.74426	8.30339	Pd	0.07028	4.85080	6.97031
C	4.14279	4.16861	8.31567	Pd	2.83319	4.88339	6.91090
C	5.47201	1.46850	8.36008	Pd	5.65681	4.88142	6.97350
O	2.10451	3.86457	11.63401	Pd	1.43718	0.82336	4.60493
O	2.08499	0.03197	12.54433	Pd	4.20407	0.82503	4.62199
O	-1.50560	5.76907	9.52745	Pd	7.02605	0.81691	4.58979
O	7.31450	4.17574	9.46124	Pd	9.82395	0.82129	4.53429
O	-0.23053	3.19455	9.48614	Pd	0.04173	3.23768	4.59330
O	8.49619	1.60083	9.48366	Pd	2.82279	3.22819	4.62975
O	5.96712	6.67190	9.45619	Pd	5.61033	3.23220	4.59975
O	1.52422	5.76305	9.48412	Pd	8.40986	3.22901	4.54527
O	4.22421	4.24859	9.49251	Pd	-1.36370	5.67987	4.61569
O	5.50956	1.46259	9.53912	Pd	1.42887	5.67131	4.58079
Pd	2.25989	1.36691	9.72169	Pd	4.22794	5.67169	4.58413
Pd	0.08240	0.02422	6.81304	Pd	7.01100	5.65697	4.52941
Pd	2.80915	0.02042	7.05627				

Pd_1_T+T+B (2)

C	2.97869	2.22387	10.86621	Pd	5.58612	0.00050	6.92229
C	0.49540	0.32936	10.93699	Pd	8.42237	0.02708	6.93738
C	-1.31361	7.04115	9.08112	Pd	-1.38891	2.44076	6.88867
C	8.23114	4.66909	8.79050	Pd	1.39742	2.41002	6.90635

C	5.79350	0.22686	8.78831	Pd	4.19044	2.42256	6.92342
C	8.45136	1.68571	8.27508	Pd	6.98979	2.43687	6.94680
C	5.48042	3.23126	8.26617	Pd	-2.78698	4.86637	6.91618
C	0.07790	3.24507	8.19501	Pd	0.00370	4.83216	6.91069
C	5.64836	6.40907	8.24625	Pd	2.79134	4.84910	6.88587
C	2.79097	4.85427	8.77098	Pd	5.58706	4.83237	6.87648
O	3.53263	2.39598	11.85698	Pd	1.40275	0.79195	4.62361
O	-4.04033	7.13139	11.92711	Pd	4.17953	0.78780	4.62234
O	-0.77419	6.28356	9.80807	Pd	6.99429	0.80693	4.58108
O	8.10777	4.54211	9.92749	Pd	9.80986	0.80175	4.55867
O	5.92423	0.38568	9.92166	Pd	-0.00402	3.23331	4.55536
O	8.48684	1.68545	9.45693	Pd	2.79727	3.23267	4.57629
O	5.46184	3.25376	9.45150	Pd	5.59613	3.22315	4.56915
O	0.10611	3.21484	9.40114	Pd	8.39260	3.23930	4.56335
O	5.57087	6.35312	9.42946	Pd	-1.41554	5.67129	4.63480
O	2.80396	4.90366	9.92241	Pd	1.39101	5.66544	4.58966
Pd	1.68351	1.28894	9.58840	Pd	4.18713	5.66836	4.57284
Pd	-4.18935	7.25920	6.98448	Pd	7.00469	5.65962	4.57248
Pd	2.79368	0.01290	7.10769				

Pd₃ line_B+B

Pd₃ line_B+B

C	3.29710	3.18623	11.22621	Pd	5.58435	0.03442	6.82851
C	2.55937	5.21350	9.01641	Pd	8.38698	0.01933	6.84491
C	6.22973	4.16961	11.14326	Pd	9.74804	2.43976	6.80574
C	7.55211	2.32644	8.91781	Pd	1.33395	2.45368	6.93363
C	-0.25985	3.15613	8.23470	Pd	4.18777	2.46063	7.11770
C	5.54109	6.58082	8.20289	Pd	7.00406	2.43710	7.01225
C	4.56851	0.88934	8.32606	Pd	-2.79757	4.87157	6.84131
C	1.34424	0.85355	8.24643	Pd	-0.02663	4.86195	7.02556
C	-1.56329	5.60543	8.26380	Pd	2.76634	4.90808	7.06241
O	3.06903	2.95531	12.34402	Pd	5.56697	4.88531	7.01702
O	2.50616	6.12252	9.76412	Pd	1.40182	0.82362	4.55937
O	6.52539	4.34527	12.25539	Pd	4.18403	0.84226	4.57717
O	7.88654	1.54837	9.73460	Pd	7.00205	0.82961	4.58231
O	-0.34197	3.08977	9.42894	Pd	9.79476	0.80586	4.53149
O	5.59922	6.67251	9.39215	Pd	0.00344	3.25597	4.54624
O	4.57054	0.74006	9.50192	Pd	2.80457	3.24488	4.66260
O	1.39767	0.92838	9.44198	Pd	5.59073	3.23646	4.67175
O	-1.69287	5.57111	9.45212	Pd	8.37265	3.24274	4.54856
Pd	2.20882	3.28887	9.41859	Pd	-1.39399	5.67611	4.55881
Pd	4.74531	3.65292	9.89137	Pd	1.40182	5.65425	4.61746
Pd	7.22144	4.26383	9.25587	Pd	4.17663	5.63447	4.60069
Pd	0.00765	0.01929	6.87316	Pd	6.96884	5.65131	4.56837
Pd	2.80028	0.02315	6.97573				

Pd₃ line_T+B

C	2.90932	3.43405	10.91863	Pd	5.58067	0.03404	6.82950
C	2.83724	5.61715	8.90229	Pd	8.42543	0.04478	6.82006
C	5.76137	4.73497	10.58426	Pd	9.77271	2.42752	6.82711
C	8.04239	2.94730	10.40917	Pd	1.39839	2.43218	6.99541
C	-0.23368	3.10951	8.25603	Pd	4.20451	2.45533	6.93085
C	9.70539	0.20409	8.33118	Pd	7.00810	2.43343	6.78547
C	4.88115	1.17994	8.30760	Pd	-2.77786	4.83814	6.96875
C	1.50093	0.84988	8.32314	Pd	0.02160	4.83565	7.05591
C	-1.44901	5.62917	8.31688	Pd	2.84430	4.96699	6.98465
O	2.95636	2.97730	11.98494	Pd	5.63229	4.84133	6.90581
O	2.82934	6.62936	9.52997	Pd	1.40022	0.81355	4.58414
O	5.90133	5.27658	11.60782	Pd	4.17471	0.81502	4.55528
O	8.47690	2.41541	11.32977	Pd	7.00968	0.79441	4.53850
O	-0.36326	2.97807	9.45827	Pd	9.82272	0.80402	4.52836
O	9.68083	0.30436	9.50094	Pd	0.02310	3.24827	4.56553
O	4.83734	1.13082	9.48780	Pd	2.79280	3.24966	4.64594
O	1.51893	0.85134	9.50478	Pd	5.58563	3.23390	4.55307
O	-1.42099	5.65250	9.50260	Pd	8.40759	3.24836	4.55065
Pd	1.63462	4.04908	9.41009	Pd	-1.38616	5.65348	4.59184
Pd	4.25766	4.05399	9.37977	Pd	1.40197	5.65145	4.61682
Pd	6.93732	3.90421	9.12195	Pd	4.20120	5.63739	4.58398
Pd	-4.18932	7.27364	6.97652	Pd	7.00524	5.65509	4.59973
Pd	-1.40996	7.26020	6.94707				

Pd₃ line_T+B+B

C	7.51499	2.32161	8.97744	Pd	-1.36937	7.27168	6.94915
C	2.64182	3.11449	10.92494	Pd	5.60075	0.02237	6.84713
C	2.75241	5.40713	8.99533	Pd	8.41570	0.01619	6.83889
C	5.36950	4.27331	11.03599	Pd	9.74749	2.41969	6.71646
C	8.27530	4.39508	10.96534	Pd	1.37122	2.38895	6.98381
C	-0.34462	3.01268	8.21493	Pd	4.19891	2.44417	6.95081
C	5.60221	6.59654	8.19212	Pd	7.01803	2.46032	7.06264
C	4.61160	1.00591	8.28177	Pd	-2.75954	4.86486	7.03536
C	1.36332	0.74960	8.27015	Pd	0.03099	4.79355	7.01747
C	-1.34018	5.63913	8.29582	Pd	2.81810	4.91781	7.03987
O	7.95406	1.55567	9.74870	Pd	5.60881	4.87183	7.05922
O	2.62465	2.56872	11.94994	Pd	1.41515	0.81576	4.55456
O	2.71244	6.38631	9.66703	Pd	4.19545	0.82378	4.55813
O	5.35991	4.52939	12.17368	Pd	7.01115	0.83785	4.59253
O	-2.31833	4.32196	11.93487	Pd	9.80268	0.79158	4.50758
O	-0.53758	2.85346	9.40509	Pd	0.02168	3.24836	4.53656
O	5.67344	6.72617	9.37746	Pd	2.79681	3.24882	4.64724

O	4.59389	0.96675	9.46807	Pd	5.60478	3.24408	4.64709
O	1.34187	0.71324	9.45226	Pd	8.36798	3.25885	4.56003
O	-1.21199	5.70677	9.47633	Pd	-1.39523	5.64992	4.59600
Pd	1.48980	3.86511	9.40278	Pd	1.41007	5.65586	4.61597
Pd	4.12092	3.77240	9.52279	Pd	4.19487	5.63152	4.59866
Pd	6.88166	4.19714	9.52232	Pd	6.99237	5.63371	4.59305
Pd	-4.17053	7.27025	6.82747				

Pd₃ line_T+T+B

C	7.40057	2.10964	10.15892	Pd	-1.40890	7.25210	6.91208
C	2.97005	3.22105	10.84315	Pd	5.58398	0.01937	6.82954
C	2.80517	5.46019	8.87437	Pd	8.40128	0.02597	6.83074
C	5.48808	4.88017	10.78829	Pd	9.74276	2.41778	6.80356
C	8.35242	4.72392	11.10979	Pd	1.37212	2.38962	6.96167
C	-0.28690	3.08615	8.24620	Pd	4.19438	2.43878	6.92638
C	9.70738	0.01989	8.32162	Pd	6.99411	2.45975	6.94667
C	4.72560	1.07872	8.28535	Pd	-2.78675	4.83958	7.07396
C	1.43144	0.79510	8.28133	Pd	0.02222	4.79372	6.99989
C	-1.35233	5.65591	8.28595	Pd	2.83520	4.91472	6.94737
O	7.50746	1.36062	11.02807	Pd	5.64895	4.83875	6.97966
O	3.03514	2.69708	11.87725	Pd	1.39217	0.80230	4.56692
O	2.71222	6.46270	9.50811	Pd	4.18084	0.80997	4.54818
O	5.31451	5.42114	11.80887	Pd	7.00793	0.81807	4.57299
O	-2.32270	4.91314	12.11265	Pd	9.80778	0.79967	4.52464
O	-0.44031	2.95017	9.44366	Pd	0.00934	3.23924	4.54912
O	9.70269	0.14987	9.48934	Pd	2.78882	3.23811	4.62499
O	4.65477	0.99606	9.46244	Pd	5.59308	3.23489	4.59512
O	1.44830	0.79176	9.46560	Pd	8.37672	3.24946	4.58129
O	-1.18175	5.74816	9.45831	Pd	-1.40289	5.64117	4.59074
Pd	1.67950	3.83440	9.36801	Pd	1.40002	5.64921	4.60130
Pd	4.32185	3.98719	9.35917	Pd	4.20199	5.63408	4.58081
Pd	7.04291	4.03017	9.75057	Pd	6.99474	5.64064	4.61541
Pd	6.99822	7.25202	6.93765				

Pd(865)_B+H

C	7.10290	2.73480	10.05612	Pd	4.81460	5.45372	6.48928
C	5.14440	5.28714	8.43617	Pd	6.84833	2.58459	8.15992
C	1.52871	4.69524	7.60384	Pd	3.64100	10.81078	7.48827
C	2.68936	7.41202	8.23619	Pd	4.72258	0.78544	7.88590
C	2.52494	11.65561	9.08625	Pd	6.85941	7.28028	6.72987
C	4.62422	9.44280	8.69057	Pd	1.54939	8.96412	7.23154
C	7.36766	8.26620	8.43594	Pd	2.07892	1.62346	8.08549
C	6.91404	11.37783	9.09285	Pd	4.20987	8.15491	7.02106

C	3.65659	1.80639	9.45573	Pd	8.40771	11.70198	7.67225
O	7.21926	2.84861	11.19543	Pd	3.15098	0.94432	5.48136
O	5.49912	5.82426	9.41780	Pd	5.24035	7.35900	4.46106
O	1.56309	4.61786	8.79927	Pd	7.39776	4.54859	6.27541
O	2.69850	7.16161	9.38707	Pd	5.78612	0.02289	5.33379
O	2.52961	11.43353	10.24353	Pd	0.51133	1.81343	5.67455
O	4.61122	9.23298	9.84723	Pd	7.90023	6.47175	4.24388
O	7.36853	8.01684	9.58682	Pd	2.60473	8.29210	4.59412
O	6.92207	11.18830	10.25271	Pd	2.59234	3.63334	6.14148
O	3.67859	1.71165	10.63258	Pd	4.73294	10.06705	4.96975
Pd	4.25613	3.46956	8.37067	Pd	5.29665	2.73059	5.81905
Pd	2.13567	6.37002	6.52415	Pd	7.36186	9.18751	4.79219
Pd	6.31407	9.91597	7.46127	Pd	2.07685	10.95331	5.14539

Pd(865)_B+B

C	5.80418	3.66052	9.67504	Pd	4.72774	5.40728	6.47108
C	2.82134	2.89548	9.80890	Pd	6.84642	2.57145	8.23278
C	1.33401	4.67885	7.58499	Pd	3.67439	10.76800	7.65824
C	3.83505	6.39125	8.01425	Pd	4.77334	0.73675	7.87715
C	1.92973	10.19281	8.87669	Pd	6.86033	7.22578	6.71257
C	5.04906	9.11045	8.62062	Pd	1.52761	9.01066	7.20719
C	7.92176	7.61149	8.35238	Pd	2.15487	1.64549	8.24844
C	6.42570	0.75533	9.26931	Pd	4.22979	8.12436	6.97338
C	3.29762	0.16818	9.24496	Pd	1.06428	11.69615	7.68903
O	6.07939	4.08274	10.72419	Pd	3.11391	0.92236	5.52966
O	2.54191	3.03545	10.92862	Pd	5.26751	7.34937	4.44170
O	1.19562	4.64036	8.77702	Pd	7.30511	4.50002	6.20237
O	3.78000	6.18421	9.18247	Pd	5.77720	0.02001	5.30569
O	1.91611	9.96999	10.03112	Pd	0.48537	1.79507	5.71288
O	5.10811	8.89556	9.77511	Pd	7.92739	6.46617	4.23675
O	7.87263	7.35360	9.49400	Pd	2.60918	8.26707	4.62763
O	6.41659	0.58535	10.43620	Pd	2.54149	3.60895	6.20096
O	4.39806	11.78430	10.40359	Pd	4.69995	10.05707	4.95133
Pd	4.23561	3.44777	8.41822	Pd	5.22023	2.72111	5.81976
Pd	2.10675	6.33606	6.61701	Pd	7.37716	9.17383	4.75861
Pd	6.28951	9.91117	7.25110	Pd	2.08038	10.94257	5.16994

Pd(865)_T+B

C	3.96950	3.63384	10.44757	Pd	4.82475	5.40929	6.51447
C	5.33289	5.14312	8.42852	Pd	6.88392	2.55482	8.08421
C	1.43923	4.61774	7.60342	Pd	3.68234	10.77873	7.57522
C	2.95573	7.15586	8.29049	Pd	4.74960	0.74204	7.91623
C	2.00779	10.38057	8.88434	Pd	6.90128	7.23926	6.70460

C	4.86895	9.53698	8.74286	Pd	1.56954	9.02411	7.24444
C	7.40412	8.21891	8.40501	Pd	2.12926	1.63142	7.97298
C	6.45810	0.97822	9.26644	Pd	4.21792	8.10799	7.03311
C	3.29955	0.85431	9.36985	Pd	8.43145	11.70801	7.68052
O	3.91553	3.82603	11.57664	Pd	3.16711	0.89930	5.47754
O	5.89461	5.71784	9.28853	Pd	5.25270	7.34134	4.46314
O	1.33474	4.44968	8.79026	Pd	7.38244	4.51008	6.20239
O	2.91623	6.96312	9.44752	Pd	5.78340	0.01146	5.34360
O	2.01836	10.17611	10.04222	Pd	0.52699	1.78893	5.63053
O	4.86520	9.30457	9.89470	Pd	7.92264	6.47031	4.24189
O	7.42905	7.98374	9.55769	Pd	2.60435	8.26866	4.62236
O	6.48463	0.85570	10.44093	Pd	2.59665	3.64817	6.14530
O	3.24293	0.61566	10.51873	Pd	4.73171	10.03070	4.96150
Pd	4.25259	3.45560	8.49690	Pd	5.22602	2.72323	5.83780
Pd	2.12977	6.34041	6.61058	Pd	7.37676	9.17929	4.77885
Pd	6.32737	9.84032	7.35729	Pd	2.09445	10.94336	5.15125

Pd(865)_T+H

C	7.32189	2.56391	10.04559	Pd	4.76663	5.41873	6.36422
C	4.68408	4.78346	9.86616	Pd	6.89584	2.55207	8.17669
C	1.47483	4.68784	7.61822	Pd	3.64822	10.78641	7.48394
C	2.70938	7.35700	8.24404	Pd	4.73898	0.80615	7.87099
C	2.56398	11.65108	9.07745	Pd	6.80846	7.22108	6.73452
C	4.61843	9.41393	8.69268	Pd	1.52327	8.91848	7.26250
C	7.33569	8.16395	8.43641	Pd	2.12251	1.62719	8.09321
C	6.90710	11.34465	9.06665	Pd	4.20721	8.10927	7.03282
C	3.72055	1.90451	9.44960	Pd	8.42396	11.68538	7.66910
O	7.50437	2.62659	11.18078	Pd	3.14318	0.93846	5.48315
O	4.93185	5.38380	10.81337	Pd	5.24052	7.38029	4.44419
O	1.45622	4.63511	8.81274	Pd	7.36283	4.53339	6.27504
O	2.71137	7.11195	9.39708	Pd	5.78277	0.02831	5.33741
O	2.55783	11.42484	10.23441	Pd	0.51242	1.80962	5.66622
O	4.59854	9.20360	9.84965	Pd	7.89589	6.47042	4.24684
O	7.29812	7.87361	9.57864	Pd	2.59902	8.28775	4.60719
O	6.91445	11.17218	10.23064	Pd	2.59243	3.62533	6.16821
O	3.72025	1.72061	10.61557	Pd	4.73435	10.06605	4.97678
Pd	4.35628	3.58670	8.36549	Pd	5.27325	2.72857	5.85999
Pd	2.12187	6.34155	6.53671	Pd	7.36107	9.18434	4.81081
Pd	6.31535	9.89031	7.47983	Pd	2.07481	10.94221	5.14798

Pd(865)_T+B+H

C	7.10110	2.57926	10.04934	Pd	6.32050	9.89765	7.43555
C	3.62072	4.24779	10.47748	Pd	4.81433	5.38372	6.53059

C	5.33910	5.19597	8.42773	Pd	6.85477	2.55131	8.14765
C	1.45235	4.67930	7.60521	Pd	3.65691	10.77439	7.47049
C	2.74462	7.32475	8.21286	Pd	4.73220	0.79604	7.86264
C	2.50488	11.55243	9.05942	Pd	6.86841	7.25253	6.74604
C	4.63748	9.38813	8.66700	Pd	1.57335	8.93448	7.20151
C	7.43271	8.28568	8.43062	Pd	2.08702	1.56995	8.12471
C	6.91062	11.31891	9.04192	Pd	4.22375	8.11181	7.00101
C	3.66270	1.58216	9.50959	Pd	8.41192	11.67679	7.63320
O	7.22494	2.62980	11.19389	Pd	3.13640	0.93230	5.48287
O	3.37229	4.58668	11.54142	Pd	5.24526	7.33822	4.47016
O	5.92876	5.80419	9.24464	Pd	7.38586	4.50997	6.21914
O	1.35104	4.64840	8.79732	Pd	5.77507	0.01541	5.31826
O	2.75790	7.07191	9.36449	Pd	0.50154	1.79949	5.66513
O	2.47715	11.29409	10.20846	Pd	7.90218	6.46865	4.24121
O	4.62746	9.17787	9.82377	Pd	2.60687	8.27539	4.58927
O	7.44932	8.08762	9.59116	Pd	2.59720	3.59634	6.22006
O	6.93460	11.13176	10.20237	Pd	4.73122	10.05065	4.95935
O	3.67123	1.24919	10.64326	Pd	5.25459	2.72382	5.86215
Pd	4.21066	3.49314	8.69965	Pd	7.35877	9.17021	4.79164
Pd	2.13930	6.32620	6.51995	Pd	2.07538	10.93830	5.12874