

Supporting Information to Manuscript entitled "Mechanism of the Oxidative Addition of Iodobenzene to Palladium(0)-Triphenylphosphine-Carbonyl complexes: a Theroretical Study"

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Additional graphical material extending this study

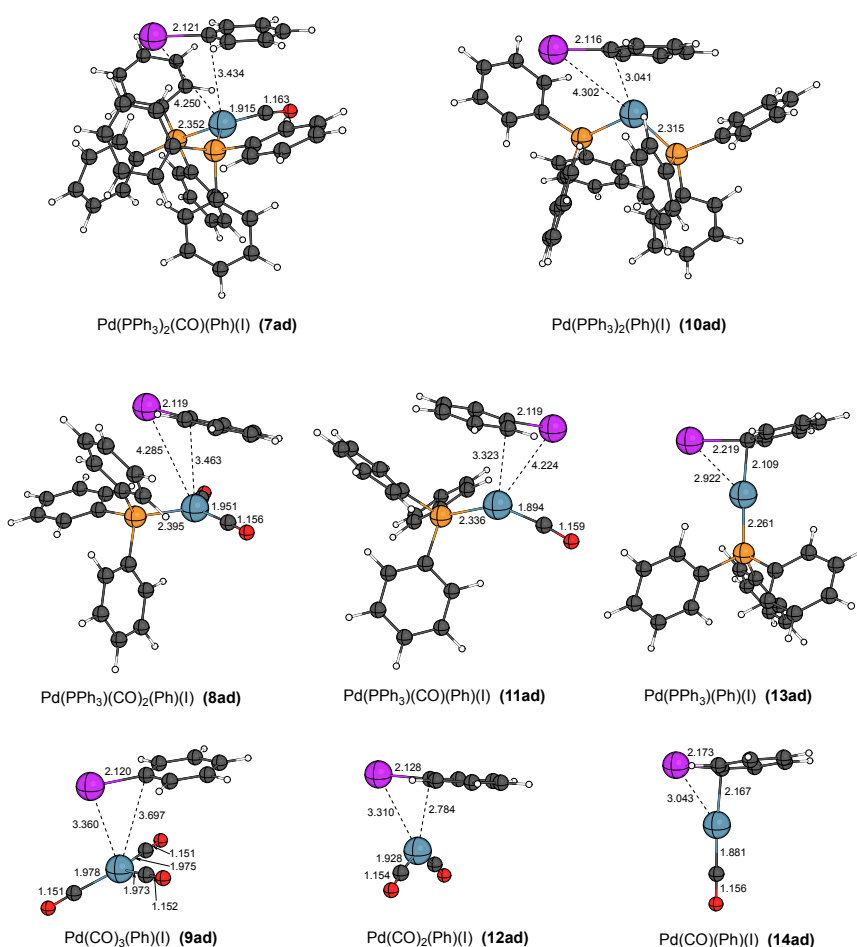


Figure S1: Computed structure of adduct for the oxidative additon of iodobenzene with tri- bis and monoligated Pd(0) complexes containing triphenylphosphine and carbonyl ligands. Bond lenthns are given in Å.

Cartesian coordinates of complexes occuring in this study

All energy values are given in a.u.

$\text{Pd}(\text{PPh}_3)_4$ (1)				P	2.03209	0.61962	1.15877
				C	2.60946	2.37606	0.97008
				C	3.59658	-0.28400	0.72126
				C	2.06049	0.45817	3.00907
				C	3.39677	5.05307	0.52941
Pd	0.00090	-0.00485	-0.00042				

C	3.38864	4.52311	1.82900	H	2.52256	-1.93113	-6.15457
C	3.00401	3.19056	2.05008	H	0.55272	-0.88099	-5.05469
C	2.62350	2.91819	-0.32965	H	3.00543	0.10569	-1.63197
C	3.01752	4.24213	-0.55272	H	4.97806	-0.89931	-2.73107
H	3.69238	6.09525	0.36043	C	1.92471	0.21813	5.82100
H	3.68643	5.14783	2.67985	C	3.03976	-0.26995	5.12176
H	3.00634	2.78604	3.06743	C	3.11330	-0.14541	3.72484
H	2.30567	2.30350	-1.17311	C	0.94667	0.94375	3.72108
H	3.00534	4.63919	-1.57374	C	0.87842	0.83363	5.11466
C	5.88110	-1.77822	-0.00862	H	1.86837	0.11291	6.91156
C	4.65648	-2.42753	0.21678	H	3.86314	-0.75028	5.66518
C	3.52519	-1.68281	0.57056	H	3.99075	-0.52492	3.19143
C	4.83177	0.35977	0.50633	H	0.11552	1.39455	3.17627
C	5.96379	-0.38454	0.13654	H	-0.00666	1.21088	5.63843
H	6.76627	-2.35463	-0.30356	C	-4.42015	-3.99680	-1.43250
H	4.56650	-3.51300	0.09482	C	-4.37652	-2.82771	-0.65570
H	2.57005	-2.19275	0.70609	C	-3.15546	-2.37283	-0.14556
H	4.91004	1.44588	0.62180	C	-2.01349	-4.25732	-1.15952
H	6.91679	0.13059	-0.03802	C	-3.23638	-4.70806	-1.68209
P	0.22828	0.48100	-2.35252	H	-5.37230	-4.34855	-1.84717
C	0.45841	2.25699	-2.85273	H	-5.28658	-2.25075	-0.45998
C	-1.18228	0.01040	-3.46915	H	-3.12679	-1.44724	0.43191
C	1.64552	-0.30053	-3.26725	H	-1.09715	-4.82105	-1.35860
C	0.71280	4.99931	-3.48806	H	-3.26167	-5.62356	-2.28575
C	1.55695	4.05248	-4.08837	P	-1.85542	1.25390	0.89925
C	1.42879	2.68822	-3.77950	C	-1.75136	3.10854	0.85940
C	-0.37984	3.21702	-2.25325	C	-2.81038	3.94181	0.44757
C	-0.26195	4.57541	-2.57052	C	-0.53100	3.69940	1.23969
H	0.81792	6.06387	-3.73041	C	-2.64082	5.33537	0.40917
H	2.32112	4.37484	-4.80725	C	-0.36469	5.08876	1.21517
H	2.08953	1.95968	-4.25982	C	-1.42020	5.91311	0.79286
H	-1.12141	2.90178	-1.51646	H	-3.76782	3.50212	0.15037
H	-0.92319	5.29802	-2.08012	H	0.30579	3.06317	1.53165
C	-3.37275	-0.81920	-5.04752	H	-3.47106	5.97170	0.07870
C	-2.85139	-1.67261	-4.06199	H	0.60098	5.51630	1.50478
C	-1.77087	-1.25461	-3.27711	H	-1.28978	7.00185	0.75516
C	-1.70245	0.85693	-4.46796	C	-3.52199	1.00089	0.11661
C	-2.79597	0.44471	-5.24617	C	-4.70361	0.77682	0.85180
H	-4.23203	-1.13350	-5.65255	C	-3.58974	1.01089	-1.29038
H	-3.29641	-2.65652	-3.88030	C	-5.92050	0.55466	0.18716
H	-1.39801	-1.90813	-2.48630	C	-4.80556	0.80613	-1.95356
H	-1.25728	1.84249	-4.63610	C	-5.97632	0.56906	-1.21520
H	-3.19749	1.11808	-6.01380	H	-4.67282	0.76850	1.94641
P	-0.38962	-2.37172	0.30535	H	-2.68017	1.16376	-1.87356
C	-0.47851	-3.01491	2.04757	H	-6.83070	0.37083	0.77156
C	0.85127	-3.54986	-0.41971	H	-4.82468	0.81095	-3.04927
C	-1.96123	-3.07916	-0.38822	H	-6.92765	0.38884	-1.73065
C	-0.53386	-3.84500	4.74895	C	-2.28706	0.98499	2.68712
C	-1.50084	-4.31154	3.84490	C	-2.28551	-0.33986	3.16342
C	-1.47283	-3.90484	2.50078	C	-2.59516	2.02870	3.58243
C	0.48717	-2.55436	2.96409	C	-2.59156	-0.62598	4.49904
C	0.46648	-2.96664	4.30159	C	-2.88833	1.74477	4.92632
H	-0.56356	-4.15994	5.79896	C	-2.89047	0.41884	5.38804
H	-2.28542	-4.99944	4.18508	H	-2.01681	-1.15220	2.48653
H	-2.23110	-4.27892	1.80547	H	-2.60356	3.06571	3.23128
H	1.25013	-1.84715	2.63418	H	-2.56970	-1.66683	4.84068
H	1.22210	-2.57707	4.99254	H	-3.12041	2.56691	5.61434
C	2.78520	-5.21314	-1.63406	H	-3.11768	0.20140	6.43862
C	2.24142	-4.13046	-2.34420	E(DMF) = -4272.023392844857; G = 0.98411324			
C	1.28770	-3.30563	-1.73654	Pd(PPh ₃) ₃ (CO) (2)			
C	1.39226	-4.64525	0.28272	Pd	0.20607	-0.01875	0.68765
C	2.35813	-5.46621	-0.32151	P	1.96126	1.42303	1.42174
H	3.54388	-5.85377	-2.10002	C	1.41895	2.72450	2.62495
H	2.56987	-3.90734	-3.36463	C	2.91656	2.36068	0.14165
H	0.88994	-2.44960	-2.28428	C	3.29859	0.58335	2.37035
H	1.06472	-4.85551	1.30543	C	0.48530	4.73583	4.37132
H	2.77644	-6.31123	0.23913	C	1.84035	4.36457	4.38201
C	3.88362	-1.48002	-4.52363	C	2.30541	3.36395	3.51645
C	2.63406	-1.47561	-5.16340				
C	1.52099	-0.88516	-4.54356				
C	2.90248	-0.31573	-2.63311				
C	4.01595	-0.89275	-3.25517				
H	4.74972	-1.94553	-5.00916				

C	0.05613	3.08077	2.64661	H	0.22484	3.67272	0.10015
C	-0.40787	4.08769	3.50530	H	1.40439	5.56414	-0.97006
H	0.12563	5.52115	5.04769	C	5.19434	-0.96491	3.77714
H	2.53836	4.85618	5.07086	C	5.46912	-0.52143	2.47542
H	3.35881	3.06391	3.54585	C	4.53214	0.25488	1.77656
H	-0.64426	2.54734	1.99561	C	3.02516	0.13032	3.68025
H	-1.47167	4.35408	3.49940	C	3.97060	-0.62830	4.38053
C	4.30147	3.67750	-1.92982	H	5.93019	-1.56862	4.32132
C	3.59827	2.49414	-2.19649	H	6.42290	-0.77774	1.99821
C	2.90310	1.84600	-1.16820	H	4.75330	0.59931	0.76215
C	3.62776	3.54723	0.40453	H	2.06263	0.37039	4.14671
C	4.31253	4.20330	-0.62793	H	3.74781	-0.96569	5.39970
H	4.82943	4.19857	-2.73745	C	-1.89481	-4.38925	-2.95854
H	3.57135	2.07915	-3.20960	C	-2.30373	-3.61660	-1.86059
H	2.32356	0.94294	-1.37924	C	-1.36457	-2.87146	-1.13839
H	3.63291	3.97631	1.41127	C	0.40499	-3.68634	-2.59029
H	4.85016	5.13543	-0.41561	C	-0.54032	-4.41939	-3.32346
P	-1.09523	1.29104	-0.85634	H	-2.63235	-4.95848	-3.53689
C	-2.52276	2.17877	-0.06425	H	-3.36253	-3.57445	-1.58047
C	-1.94137	0.34917	-2.20057	H	-1.67933	-2.23512	-0.30203
C	-0.29547	2.69322	-1.77026	H	1.46095	-3.72108	-2.87922
C	-4.69174	3.47746	1.19145	H	-0.21487	-5.01791	-4.18358
C	-4.12595	4.01609	0.02451	C	-0.66534	-0.65953	2.29723
C	-3.05154	3.36932	-0.60332	O	-0.99603	-1.04537	3.34363
C	-3.10027	1.64143	1.10197	E(DMF)= -3349.334555880666; G= 0.73691434			
C	-4.18029	2.28421	1.72510	Pd(PPh ₃) ₂ (CO) ₂ (3)			
H	-5.52880	3.98709	1.68330	Pd	-0.06455	-1.95302	-0.01295
H	-4.52190	4.94647	-0.39913	H	-0.02813	0.89042	-5.29560
H	-2.61886	3.79344	-1.51516	H	0.66331	3.20949	-4.64573
H	-2.68682	0.72005	1.52478	H	-5.64444	-0.45082	-3.91370
H	-4.61551	1.85537	2.63526	C	-0.20554	1.25201	-4.27568
C	-3.10831	-1.23047	-4.23116	C	0.18196	2.55250	-3.91230
C	-1.71240	-1.10028	-4.15620	H	2.85557	0.82858	-3.87601
C	-1.13789	-0.33174	-3.13898	H	-6.29814	-2.77535	-3.25608
C	-3.34055	0.21424	-2.28320	H	-1.09477	-0.61181	-3.62489
C	-3.91670	-0.57857	-3.28900	C	-5.05122	-0.99947	-3.17193
H	-3.56291	-1.84993	-5.01357	C	-0.81029	0.40650	-3.33737
H	-1.06945	-1.62662	-4.87081	H	4.53017	2.56913	-3.20535
H	-0.04964	-0.25205	-3.06043	H	-3.64175	0.62037	-2.89455
H	-3.98240	0.72944	-1.56101	C	-5.41761	-2.30430	-2.80360
H	-5.00822	-0.68208	-3.33669	C	-3.92750	-0.39281	-2.59401
P	1.15391	-1.92938	-0.42655	C	3.05488	1.02493	-2.81700
C	1.75094	-3.22681	0.76135	O	0.61977	-3.33434	-2.71198
C	2.66696	-1.70607	-1.46694	C	-0.04265	3.00118	-2.60325
C	0.00003	-2.90388	-1.49151	C	3.98791	2.00037	-2.44063
C	2.78879	-5.10490	2.59182	H	0.26487	4.01083	-2.30726
C	2.41868	-5.50916	1.29816	C	-4.64995	-3.00480	-1.86112
C	1.90616	-4.57610	0.38586	C	-1.05592	0.85767	-2.02166
C	2.11195	-2.83180	2.06213	H	1.61743	-0.44821	-2.12650
C	2.63608	-3.76325	2.97053	C	-3.15511	-1.08996	-1.64322
H	3.19027	-5.83707	3.30287	H	-4.92513	-4.02661	-1.57561
H	2.53116	-6.55792	0.99699	C	2.35806	0.30322	-1.83700
H	1.61998	-4.90235	-0.61902	C	-0.65983	2.16195	-1.66440
H	1.98507	-1.78784	2.35846	C	0.40611	-2.85995	-1.67551
H	2.92246	-3.43115	3.97415	C	-3.51994	-2.40293	-1.28767
C	4.99435	-0.97510	-2.90834	C	4.22944	2.24774	-1.07812
C	3.73559	-0.93191	-3.52806	H	4.96242	3.00706	-0.77785
C	2.58363	-1.28674	-2.81345	P	-1.70187	-0.33606	-0.77980
C	3.93962	-1.76572	-0.86102	H	-3.51924	2.06010	-0.94203
C	5.08883	-1.39681	-1.57378	H	-0.84147	2.52198	-0.64779
H	5.89415	-0.68418	-3.46245	H	-2.90183	-2.94982	-0.56454
H	3.64685	-0.61429	-4.57395	C	2.59376	0.54511	-0.47270
H	1.61042	-1.24543	-3.31214	C	3.54213	1.52028	-0.09876
H	4.03086	-2.09074	0.17932	C	-3.36759	1.81379	0.11455
H	6.06685	-1.44138	-1.07859	C	-2.53217	0.73644	0.47760
C	1.05711	4.85345	-2.99432	H	2.74828	-3.13046	0.50955
C	0.47883	3.84584	-3.77788	H	1.08855	2.46430	0.66142
C	-0.20170	2.77667	-3.17202				
C	0.28747	3.71572	-0.99114				
C	0.94817	4.78931	-1.59615				
H	1.59331	5.68427	-3.46850				
H	0.54859	3.89026	-4.87223				
H	-0.66866	2.01330	-3.80153				

H	3.74293	1.71490	0.96047
P	1.68083	-0.46812	0.77597
H	-4.64477	3.41844	0.80858
C	-4.00282	2.57826	1.10105
C	3.37619	-2.63819	1.26291
C	-0.60091	-2.84561	1.63778
C	0.84200	2.10646	1.66522
H	4.69055	-4.33968	1.53040
C	-2.35563	0.43288	1.83851
C	3.07016	-1.31953	1.65191
H	-1.70024	-0.39635	2.11996
C	1.10730	0.76721	2.01297
C	4.45971	-3.31459	1.84235
H	0.06230	4.02127	2.30977
C	-3.82224	2.26759	2.45982
O	-0.84902	-3.31443	2.66921
C	0.27161	2.98454	2.59887
C	-3.00143	1.19205	2.82508
C	3.85249	-0.69322	2.64296
C	5.23785	-2.68449	2.82551
H	3.61064	0.32386	2.96782
H	-4.32170	2.86672	3.23045
C	0.78516	0.32365	3.31487
C	4.92878	-1.37515	3.22772
H	0.96658	-0.72044	3.59389
H	6.08123	-3.21467	3.28366
H	-2.84843	0.94673	3.88169
C	-0.02924	2.54172	3.89441
C	0.23364	1.20821	4.24967
H	5.52909	-0.88158	4.00177
H	-0.47360	3.22926	4.62317
H	-0.00344	0.85109	5.25884

E(DMF)= -2426.651698366113; G= 0.48838738

Pd(PPh₃)(CO)₃ (4)

Pd	0.46672	-2.71482	-0.78474
P	0.48259	-0.35492	-0.17778
H	-0.76591	1.16208	-4.72884
H	-2.19407	3.06598	-3.94707
C	-0.88960	1.35351	-3.65603
C	-1.69061	2.42096	-3.21750
H	0.35215	-0.32610	-3.06170
C	-0.25652	0.52148	-2.72401
O	3.19648	-2.91154	-2.30873
O	-2.13212	-2.82141	-2.53185
C	-1.85047	2.65552	-1.84332
C	2.17882	-2.91426	-1.76516
C	-1.17077	-2.85522	-1.89502
H	-2.47588	3.48714	-1.49622
C	-0.40694	0.75860	-1.34201
H	1.63676	2.32108	-0.93956
C	-1.20938	1.83116	-0.90621
H	3.92535	3.27403	-0.66760
C	2.42790	1.71944	-0.47911
C	3.71559	2.25484	-0.32267
C	2.15114	0.40954	-0.04202
H	-1.33175	2.02092	0.16606
C	4.73068	1.49189	0.27466
H	5.73559	1.91329	0.39632
C	3.17765	-0.35710	0.54722
C	4.45884	0.18506	0.71113
H	2.96428	-1.38312	0.86959
C	0.37551	-3.58073	0.99791
H	-1.96282	-1.30041	1.02324
H	5.25062	-0.41766	1.17113
C	-0.29299	0.02121	1.44839
C	-1.52263	-0.60231	1.74644
O	0.31276	-3.96644	2.08321
H	1.24118	1.38187	2.16665

C	0.28496	0.89687	2.38774
C	-2.17266	-0.33842	2.95824
H	-3.13102	-0.82244	3.17842
C	-0.36288	1.14640	3.60748
C	-1.59212	0.53464	3.89321
H	0.09634	1.82381	4.33755
H	-2.09612	0.73232	4.84654

E(DMF)= -1503.966376355896; G= 0.23489165

Pd(CO)₄ (5)

Pd	0.00000	0.00000	0.00000
C	1.16318	-1.16318	1.16318
C	1.16318	1.16318	-1.16318
C	-1.16318	-1.16318	-1.16318
C	-1.16318	1.16318	1.16318
O	1.82619	-1.82619	1.82619
O	1.82619	1.82619	-1.82619
O	-1.82619	-1.82619	-1.82619
O	-1.82619	1.82619	1.82619

E(DMF)= -581.280867743781; G= -0.01224386

Pd(PPh₃)₃ (6)

Pd	0.61381	0.18923	0.12208
P	2.09592	1.51001	1.33651
C	1.47131	2.74183	2.56907
C	3.01855	2.54454	0.10353
C	3.45928	0.67779	2.26364
C	0.39112	4.66917	4.32465
C	1.76084	4.35818	4.37434
C	2.29907	3.39928	3.50390
C	0.09560	3.04385	2.54417
C	-0.44214	4.00720	3.41048
H	-0.02579	5.42164	5.00552
H	2.41309	4.86699	5.09494
H	3.36585	3.15230	3.55536
H	-0.55340	2.50980	1.84275
H	-1.51508	4.23037	3.36993
C	4.29495	4.03608	-1.92317
C	3.80701	2.74995	-2.19826
C	3.16584	2.01339	-1.19489
C	3.51892	3.83155	0.37531
C	4.14924	4.57343	-0.63496
H	4.77766	4.62346	-2.71343
H	3.90712	2.32142	-3.20223
H	2.75312	1.02276	-1.41612
H	3.39691	4.27037	1.37062
H	4.51968	5.58173	-0.41489
P	-1.00422	1.32866	-1.07363
C	-2.38151	1.98560	-0.03365
C	-1.89675	0.41484	-2.40798
C	-0.39556	2.83990	-1.95297
C	-4.39483	2.92104	1.70571
C	-3.99171	3.69954	0.60939
C	-2.99435	3.23301	-0.26059
C	-2.79013	1.20936	1.07166
C	-3.79535	1.67075	1.93159
H	-5.17348	3.28797	2.38561
H	-4.45703	4.67605	0.42917
H	-2.68379	3.84354	-1.11587
H	-2.29060	0.25063	1.26317
H	-4.10194	1.05964	2.78910
C	-3.10925	-1.11931	-4.44419
C	-1.70974	-1.01206	-4.38320

C	-1.11182	-0.26477	-3.36386
C	-3.29831	0.30712	-2.47845
C	-3.89827	-0.46468	-3.48753
H	-3.58167	-1.72335	-5.22822
H	-1.08383	-1.53927	-5.11233
H	-0.02013	-0.20674	-3.29081
H	-3.92287	0.82647	-1.74360
H	-4.99188	-0.54959	-3.52656
P	1.15425	-1.99318	-0.41169
C	1.51971	-3.23194	0.91221
C	2.75413	-1.90543	-1.33337
C	0.03274	-2.93952	-1.53257
C	2.18455	-5.00429	3.00198
C	1.60899	-5.49226	1.81741
C	1.28222	-4.61342	0.77331
C	2.07834	-2.74603	2.11194
C	2.42174	-3.62798	3.14535
H	2.44348	-5.69576	3.81307
H	1.41429	-6.56603	1.70357
H	0.83887	-5.00254	-0.14960
H	2.25216	-1.67075	2.22338
H	2.87130	-3.23061	4.06252
C	5.20099	-1.37957	-2.65360
C	3.98078	-1.08325	-3.28401
C	2.77014	-1.33833	-2.62834
C	3.98232	-2.21519	-0.71591
C	5.19390	-1.94862	-1.37152
H	6.14995	-1.16757	-3.15983
H	3.97155	-0.64305	-4.28802
H	1.82456	-1.08993	-3.12067
H	3.99319	-2.64754	0.28870
H	6.13998	-2.18651	-0.87058
C	0.71284	5.13597	-3.16864
C	0.05847	4.17082	-3.94683
C	-0.50057	3.03184	-3.34381
C	0.26613	3.81672	-1.17818
C	0.80566	4.95860	-1.77826
H	1.15240	6.02221	-3.64184
H	-0.02621	4.30382	-5.03278
H	-1.02037	2.29234	-3.96160
H	0.36332	3.67509	-0.09829
H	1.32253	5.70035	-1.15937
C	5.36341	-0.95173	3.57470
C	5.56953	-0.54763	2.24661
C	4.62963	0.26344	1.59522
C	3.25576	0.26367	3.59918
C	4.20402	-0.53656	4.25029
H	6.10105	-1.58609	4.08040
H	6.47078	-0.86643	1.70889
H	4.79960	0.56319	0.55636
H	2.34301	0.56312	4.12759
H	4.03270	-0.84357	5.28921
C	-1.82396	-4.32782	-3.13510
C	-2.27395	-3.51023	-2.08608
C	-1.35179	-2.81047	-1.30019
C	0.47829	-3.76668	-2.58118
C	-0.44830	-4.45015	-3.38401
H	-2.54565	-4.85912	-3.76707
H	-3.34791	-3.39155	-1.90139
H	-1.69711	-2.13239	-0.50986
H	1.55249	-3.87559	-2.77017
H	-0.09203	-5.08441	-4.20571

E(DMF)= -3236.009855100910; G= 0.73101860

Pd(PPh₃)₂(CO) (7)

Pd	-0.07742	-1.28611	-0.98394
P	1.89542	-0.12814	-0.38547
P	-1.91854	-0.19847	0.02125
C	1.84305	1.70695	-0.20136

C	2.45468	2.56761	-1.13344
C	1.06904	2.26752	0.83887
C	2.31297	3.95951	-1.01463
H	3.04774	2.15023	-1.95449
C	0.94867	3.65478	0.96710
H	0.55639	1.61331	1.55153
C	1.56876	4.50729	0.03927
H	2.79490	4.61621	-1.74927
H	0.34681	4.07215	1.78196
H	1.45959	5.59470	0.13250
C	3.38383	-0.37522	-1.45778
C	3.21507	-0.94137	-2.73412
C	4.67430	-0.00215	-1.03010
C	4.32112	-1.12539	-3.57885
H	2.21046	-1.24689	-3.05167
C	5.77794	-0.19059	-1.87223
H	4.81312	0.43634	-0.03590
C	5.60276	-0.75130	-3.14898
H	4.18029	-1.56795	-4.57184
H	6.77923	0.10000	-1.53220
H	6.46819	-0.90031	-3.80590
C	2.50682	-0.70721	1.26301
C	2.34250	-2.07780	1.55846
C	3.08510	0.13761	2.23019
C	2.74305	-2.59085	2.79919
H	1.87554	-2.73209	0.81148
C	3.47798	-0.37714	3.47571
H	3.21711	1.20317	2.01606
C	3.30660	-1.73985	3.76444
H	2.60177	-3.65594	3.01835
H	3.91868	0.29235	4.22445
H	3.60974	-2.13767	4.74009
C	-2.07867	-0.42226	1.84968
C	-3.32093	-0.40853	2.51535
C	-0.90061	-0.61537	2.59929
C	-3.37597	-0.56570	3.90852
H	-4.24561	-0.28022	1.94133
C	-0.95662	-0.76770	3.99146
H	0.06413	-0.66706	2.08552
C	-2.19616	-0.74177	4.64972
H	-4.34743	-0.55481	4.41825
H	-0.02782	-0.92165	4.55308
H	-2.24595	-0.87169	5.73775
C	-3.59969	-0.69416	-0.57178
C	-3.84756	-2.07427	-0.72189
C	-4.62111	0.22566	-0.87630
C	-5.10313	-2.52692	-1.14563
H	-3.03964	-2.78818	-0.51762
C	-5.87474	-0.23069	-1.31575
H	-4.43816	1.30105	-0.77372
C	-6.12041	-1.60507	-1.44615
H	-5.28541	-3.60295	-1.25665
H	-6.66177	0.49373	-1.55821
H	-7.09891	-1.95967	-1.79125
C	-1.94829	1.63516	-0.19122
C	-1.38981	2.15179	-1.37791
C	-2.49452	2.52037	0.75721
C	-1.39457	3.53023	-1.62197
H	-0.93186	1.46116	-2.09705
C	-2.49339	3.90204	0.51302
H	-2.91490	2.12864	1.68963
C	-1.94816	4.40826	-0.67680
H	-0.94590	3.92257	-2.54155
H	-2.91506	4.58653	1.25914
H	-1.93978	5.48941	-0.86109
C	-0.14708	-2.86102	-2.07104
O	-0.18428	-3.83387	-2.70478

E(DMF)= -2313.330543542690; G= 0.48280857

Pd(PPh₃)(CO)₂ (8)

Pd	2.19175	0.22861	-0.26144
P	-0.17839	-0.03509	-0.07760
C	-1.06284	-1.05412	-1.33523
C	-2.33240	-0.71260	-1.84021
C	-0.43431	-2.23375	-1.78447
C	-2.96558	-1.54491	-2.77594
H	-2.82519	0.20486	-1.50323
C	-1.07595	-3.06974	-2.70764
H	0.56305	-2.48957	-1.40933
C	-2.34238	-2.72540	-3.20746
H	-3.95147	-1.26881	-3.16735
H	-0.58159	-3.98752	-3.04655
H	-2.83978	-3.37439	-3.93816
C	-1.12976	1.54231	-0.05777
C	-2.29943	1.70936	0.70989
C	-0.66473	2.60816	-0.85374
C	-2.99677	2.92640	0.67516
H	-2.66132	0.88576	1.33540
C	-1.36604	3.82167	-0.88956
H	0.25727	2.48439	-1.43544
C	-2.53268	3.98265	-0.12475
H	-3.90627	3.04904	1.27514
H	-0.99565	4.64817	-1.50750
H	-3.07671	4.93450	-0.14728
C	-0.65740	-0.82094	1.51944
C	-1.51994	-1.93037	1.60290
C	-0.11435	-0.27441	2.70244
C	-1.83710	-2.48173	2.85439
H	-1.94528	-2.36244	0.69158
C	-0.44339	-0.82087	3.94870
H	0.56401	0.58523	2.63976
C	-1.30431	-1.92836	4.02746
H	-2.50607	-3.34893	2.91057
H	-0.02046	-0.38613	4.86170
H	-1.55524	-2.36091	5.00286
C	3.12921	-1.09377	-1.33540
O	3.64425	-1.91350	-1.96772
C	2.74361	1.79564	0.75533
O	2.98289	2.72940	1.39319

E(DMF)= -1390.645366204629; G= 0.23390552

Pd(CO)₃ (9)

Pd	0.37479	0.37341	0.37414
C	1.20197	-1.22381	1.19917
C	1.19293	1.19496	-1.22851
C	-1.23010	1.18979	1.19175
O	1.69390	-2.13497	1.69834
O	1.68404	1.68813	-2.14342
O	-2.14654	1.68348	1.67952

E(DMF)= -467.961821279579; G= -0.01338656

Pd(PPh₃)₂ (10)

Pd	-0.00234	0.04207	-0.78424
P	-2.23884	0.00195	-0.37719
P	2.23321	0.02983	-0.37313
C	-2.55151	-0.21501	1.43304
C	-3.59974	-1.00390	1.94474
C	-1.68074	0.44100	2.32845
C	-3.77313	-1.13269	3.33226
H	-4.27835	-1.52252	1.25835
C	-1.86051	0.31613	3.71222
H	-0.84660	1.02924	1.92503
C	-2.90643	-0.47422	4.21785

H	-4.58959	-1.75308	3.72269
H	-1.17031	0.82450	4.39600
H	-3.04081	-0.58284	5.30132
C	-3.25364	-1.34857	-1.12405
C	-2.66238	-2.62645	-1.21239
C	-4.56876	-1.16307	-1.59087
C	-3.38288	-3.70419	-1.74344
H	-1.62931	-2.76154	-0.86677
C	-5.28429	-2.24338	-2.13166
H	-5.03557	-0.17329	-1.53263
C	-4.69586	-3.51471	-2.20586
H	-2.91508	-4.69437	-1.80703
H	-6.30709	-2.08889	-2.49513
H	-5.25656	-4.35661	-2.62912
C	-3.20571	1.52012	-0.78732
C	-2.91625	2.16148	-2.00920
C	-4.20297	2.05209	0.05259
C	-3.62524	3.30718	-2.39286
H	-2.12130	1.75789	-2.64980
C	-4.90329	3.20680	-0.32905
H	-4.42938	1.56350	1.00654
C	-4.61888	3.83413	-1.55149
H	-3.39469	3.79778	-3.34599
H	-5.67479	3.61813	0.33353
H	-5.16464	4.73876	-1.84491
C	3.23470	1.48186	-0.92244
C	4.52444	1.37187	-1.47624
C	2.65703	2.75911	-0.76150
C	5.22827	2.52526	-1.85814
H	4.97905	0.38410	-1.60784
C	3.36724	3.90818	-1.13162
C	1.64348	2.83850	-0.34841
C	4.65464	3.79356	-1.68327
H	6.23097	2.43072	-2.29130
H	2.91200	4.89707	-0.99807
H	5.20680	4.69254	-1.98171
C	3.21488	-1.40568	-0.99328
C	2.90972	-1.89199	-2.28129
C	4.24293	-2.01752	-0.25007
C	3.63381	-2.96167	-2.82461
H	2.09152	-1.42750	-2.84627
C	4.95881	-3.09605	-0.79220
H	4.48208	-1.65125	0.75376
C	4.65885	-3.56755	-2.07936
H	3.39041	-3.33108	-3.82759
H	5.75468	-3.57022	-0.20498
H	5.21740	-4.41258	-2.49938
C	2.55197	-0.00076	1.44979
C	1.66232	-0.73774	2.25852
C	3.63060	0.67676	2.05135
C	1.85385	-0.80407	3.64494
H	0.80574	-1.23684	1.78850
C	3.81733	0.61240	3.44140
H	4.32344	1.25860	1.43288
C	2.93175	-0.12773	4.24011
H	1.14852	-1.37331	4.26233
H	4.65855	1.14473	3.90233
H	3.07781	-0.17253	5.32660

E(DMF)= -2199.995288184945; G= 0.47745400

Pd(PPh₃)(CO) (11)

Pd	0.05960	0.03591	-0.91523
P	-2.21289	-0.01180	-0.32188
C	-2.54273	-0.23232	1.47661
C	-3.62140	-0.99509	1.96329
C	-1.68613	0.42142	2.38607
C	-3.84426	-1.09394	3.34533
H	-4.28573	-1.51258	1.26242
C	-1.91716	0.32626	3.76489

H	-0.83334	0.99651	2.00276
C	-2.99655	-0.43231	4.24679
H	-4.68516	-1.69080	3.71927
H	-1.24617	0.83709	4.46542
H	-3.17208	-0.51404	5.32647
C	-3.19116	-1.35909	-1.10951
C	-2.57991	-2.62334	-1.23830
C	-4.51323	-1.17765	-1.55842
C	-3.28921	-3.69522	-1.79593
H	-1.54236	-2.75579	-0.90647
C	-5.21722	-2.25284	-2.12264
H	-4.99235	-0.19611	-1.46936
C	-4.60895	-3.51177	-2.23980
H	-2.80655	-4.67494	-1.89477
H	-6.24534	-2.10401	-2.47253
H	-5.16020	-4.34939	-2.68320
C	-3.15316	1.51294	-0.75007
C	-2.87814	2.12179	-1.99192
C	-4.12995	2.07096	0.09639
C	-3.58233	3.26618	-2.38693
H	-2.10154	1.69582	-2.64024
C	-4.82594	3.22336	-0.29962
H	-4.34426	1.60683	1.06500
C	-4.55612	3.82065	-1.54000
H	-3.36315	3.73348	-3.35397
H	-5.58172	3.65654	0.36674
H	-5.09786	4.72402	-1.84387
C	1.88695	0.07554	-1.38260
O	3.00695	0.10192	-1.66639

E(DMF)= -1277.319955155192; G= 0.23041283

Pd(CO)₂ (12)

Pd	-0.00859	-0.33740	-0.00859
C	1.33268	0.09766	-1.32770
C	-1.32770	0.09766	1.33268
O	2.10674	0.48907	-2.08182
O	-2.08182	0.48907	2.10674

E(DMF)= -354.632136965832; G= -0.01436713

Pd(PPh₃) (13)

Pd	0.45521	0.97199	0.64466
P	-1.19185	-0.43438	0.47158
C	-0.77762	-2.07767	-0.27086
C	-1.63316	-2.74583	-1.16837
C	0.43400	-2.68853	0.11177
C	-1.27958	-4.00739	-1.67207
H	-2.57788	-2.28283	-1.47155
C	0.77803	-3.95276	-0.38314
H	1.10674	-2.15435	0.79509
C	-0.07753	-4.61485	-1.27961
H	-1.95046	-4.51843	-2.37359
H	1.72204	-4.41881	-0.07709
H	0.19548	-5.60020	-1.67446
C	-2.61069	0.12416	-0.57642
C	-2.31210	0.72989	-1.81477
C	-3.95634	-0.05711	-0.20494
C	-3.34219	1.13115	-2.67415
H	-1.26201	0.88750	-2.09208
C	-4.98707	0.35952	-1.06299
H	-4.20184	-0.52379	0.75459
C	-4.68437	0.94935	-2.29899
H	-3.09803	1.59549	-3.63691
H	-6.03260	0.21801	-0.76246
H	-5.49090	1.27287	-2.96750

C	-2.02300	-0.90876	2.05452
C	-2.25327	0.10420	3.00832
C	-2.45702	-2.22128	2.32313
C	-2.91999	-0.18844	4.20518
H	-1.89551	1.12105	2.80292
C	-3.11445	-2.51333	3.52879
H	-2.28162	-3.01476	1.58880
C	-3.34951	-1.49987	4.46977
H	-3.09684	0.60656	4.93975
H	-3.44664	-3.53879	3.73082
H	-3.86124	-1.73164	5.41140

E(DMF)= -1163.955297465773; G= 0.22474168

Pd(CO) (14)

Pd	-1.56954	0.40979	-0.41521
C	-0.16270	0.51925	-1.58592
O	0.73287	0.56669	-2.31675

E(DMF)= -241.277888790670; G= -0.01573840

Pd(PPh₃)₂(CO)(PhI) (7ad)

Pd	0.10131	0.61930	-0.79408
P	-1.70937	-0.59812	0.08573
P	2.10057	-0.54464	-0.36885
C	-1.65852	-2.16039	-0.89251
C	-2.35603	-2.27028	-2.11207
C	-0.76004	-3.18388	-0.52027
C	-2.15639	-3.38345	-2.94389
H	-3.04784	-1.47633	-2.41498
C	-0.56954	-4.29604	-1.34988
H	-0.19614	-3.10252	0.41208
C	-1.26391	-4.39970	-2.56639
H	-2.70137	-3.45364	-3.89286
H	0.13812	-5.07693	-1.04696
H	-1.10632	-5.26601	-3.21999
C	-3.41218	0.05907	-0.24596
C	-3.54368	1.12201	-1.16016
C	-4.56535	-0.46473	0.37172
C	-4.80971	1.64570	-1.46282
H	-2.63933	1.53366	-1.62329
C	-5.82887	0.06453	0.07334
H	-4.47649	-1.28497	1.09275
C	-5.95423	1.11953	-0.84538
H	-4.90004	2.47282	-2.17778
H	-6.72011	-0.34773	0.56117
H	-6.94337	1.53324	-1.07476
C	-1.85203	-1.17741	1.83496
C	-1.45378	-0.27767	2.84289
C	-2.32693	-2.45070	2.20654
C	-1.52859	-0.63565	4.19487
H	-1.05051	0.69981	2.56095
C	-2.39388	-2.81380	3.55992
H	-2.63356	-3.16575	1.43564
C	-1.99686	-1.90887	4.55699
H	-1.20461	0.07657	4.96287
H	-2.75753	-3.81036	3.83760
H	-2.04776	-2.19770	5.61392
C	2.13151	-1.92018	0.86303
C	1.54536	-1.66838	2.12086
C	2.59698	-3.21657	0.57017
C	1.41632	-2.69262	3.06611
H	1.16427	-0.66643	2.34217
C	2.46085	-4.24479	1.51642
H	3.04341	-3.42827	-0.40650
C	1.86713	-3.98840	2.76210

H	0.93538	-2.48297	4.02773
H	2.81672	-5.25367	1.27504
H	1.74976	-4.79726	3.49340
C	3.54172	0.49859	0.11441
C	3.71092	1.71877	-0.57311
C	4.42994	0.16409	1.15360
C	4.75633	2.58506	-0.23070
H	2.99943	1.98802	-1.36330
C	5.46551	1.04407	1.50700
H	4.30556	-0.77986	1.69519
C	5.63196	2.25447	0.81763
H	4.88037	3.52921	-0.77491
H	6.14603	0.78206	2.32665
H	6.43925	2.94202	1.09721
C	2.67639	-1.37789	-1.91016
C	1.69917	-1.88202	-2.79290
C	4.04083	-1.54962	-2.21509
C	2.08255	-2.56313	-3.95634
H	0.63820	-1.73238	-2.56484
C	4.42065	-2.22044	-3.38768
H	4.80442	-1.15842	-1.53365
C	3.44370	-2.73101	-4.25753
H	1.31292	-2.95535	-4.63093
H	5.48497	-2.34600	-3.62252
H	3.74495	-3.25288	-5.17386
C	0.05006	1.80432	-2.29732
O	0.07625	2.35500	-3.32129
C	-0.86687	4.71134	-0.90674
C	0.52898	4.81940	-0.80898
C	-1.57346	3.94805	0.03270
H	1.08960	5.40255	-1.54929
H	-2.66184	3.83975	-0.04261
C	1.22336	4.17442	0.22546
C	-0.89448	3.29130	1.07095
H	2.31191	4.25346	0.30126
H	-1.45485	2.69917	1.79945
C	0.50136	3.41494	1.15977
I	1.55014	2.47390	2.74467
H	-1.39991	5.20929	-1.72448

E(DMF)= -2842.650523185504; G= 0.56640567

Pd(PPh₃)₂(CO)₂(PhI) (8ad)

Pd	-1.01891	1.44957	0.54868
P	1.12409	0.40081	0.34441
C	1.21285	-0.95766	-0.89505
C	1.50601	-2.28978	-0.54706
C	0.88538	-0.65201	-2.23410
C	1.48296	-3.29679	-1.52491
H	1.74853	-2.54280	0.48941
C	0.88155	-1.65555	-3.20932
H	0.62928	0.37732	-2.50918
C	1.17680	-2.98369	-2.85738
H	1.70764	-4.33125	-1.23979
H	0.63226	-1.40259	-4.24667
H	1.16241	-3.77177	-3.61941
C	1.96955	-0.29651	1.83124
C	3.32183	-0.69485	1.79202
C	1.24459	-0.42980	3.02871
C	3.93138	-1.23348	2.93281
H	3.89816	-0.58115	0.86735
C	1.85672	-0.96933	4.17089
H	0.19894	-0.10741	3.05817
C	3.19856	-1.37383	4.12378
H	4.98259	-1.54235	2.89468
H	1.28152	-1.07127	5.09901
H	3.67738	-1.79396	5.01641
C	2.37194	1.61309	-0.27774
C	3.40953	1.26859	-1.16640
C	2.27623	2.94012	0.18980

C	4.33963	2.23659	-1.57468
H	3.48390	0.24539	-1.54997
C	3.21132	3.90294	-0.21409
H	1.45509	3.21400	0.86481
C	4.24478	3.55336	-1.09837
H	5.14143	1.95940	-2.27019
H	3.12715	4.93176	0.15534
H	4.97093	4.30869	-1.42170
C	-1.45849	2.17892	-1.20621
O	-1.63586	2.59635	-2.26971
C	-1.79399	1.69004	2.30897
O	-2.23058	1.83467	3.37114
C	-3.64696	-0.32873	-2.17017
C	-4.09740	-0.02964	-0.87605
C	-3.53729	-0.67300	0.23904
C	-2.52525	-1.62687	0.03814
C	-2.06313	-1.93660	-1.24943
C	-2.62963	-1.27741	-2.35059
H	-4.07852	0.18713	-3.03471
H	-4.87990	0.72199	-0.72086
H	-3.88620	-0.43555	1.24789
H	-1.26535	-2.66912	-1.39582
H	-2.25915	-1.50881	-3.35564
I	-1.68588	-2.61992	1.71120

E(DMF)= -2842.650523185504; G= 0.56640567

Pd(CO)₃(PhI) (9ad)

Pd	0.28310	1.11384	-0.01186
C	-0.03248	2.22147	-1.61431
O	-0.22625	2.88992	-2.53175
C	-0.29585	1.83451	1.73349
O	-0.63035	2.28074	2.74031
C	-4.34618	3.95608	0.58512
C	-3.96938	3.63697	-0.72841
C	-3.49581	2.35345	-1.04128
C	-3.40350	1.39729	-0.01860
C	-3.77999	1.69658	1.29921
C	-4.25227	2.98537	1.59337
H	-4.03843	4.39069	-1.52176
H	-3.19215	2.10956	-2.06375
H	-3.69593	0.94308	2.08878
H	-4.54434	3.22689	2.62200
I	-2.61718	-0.52116	-0.46232
C	1.54908	-0.40415	-0.08233
O	2.32477	-1.25376	-0.11447
H	-4.71310	4.96078	0.82276

E(DMF)= -997.278851177027; G= 0.06643265

Pd(PPh₃)₂(PhI) (10ad)

Pd	0.01481	0.81390	-0.54345
P	-1.79281	-0.61909	-0.34526
P	2.10459	-0.17453	-0.43704
C	-1.76310	-2.26927	-1.16830
C	-2.73778	-2.70524	-2.08642
C	-0.65595	-3.10286	-0.89432
C	-2.59749	-3.94558	-2.73030
H	-3.60992	-2.07695	-2.29656
C	-0.52797	-4.34467	-1.52579
H	0.10976	-2.77342	-0.18511
C	-1.49494	-4.76826	-2.45366
H	-3.36202	-4.27173	-3.44651
H	0.33903	-4.97736	-1.30090
H	-1.39062	-5.73649	-2.95715

C	-3.42094	0.09133	-0.83390
C	-3.54353	0.59887	-2.14651
C	-4.47977	0.28256	0.07394
C	-4.70680	1.26611	-2.54738
H	-2.70468	0.48767	-2.84556
C	-5.63640	0.97384	-0.32302
H	-4.39366	-0.09744	1.09697
C	-5.75638	1.46348	-1.63165
H	-4.78966	1.65200	-3.57048
H	-6.44936	1.12860	0.39710
H	-6.66041	2.00265	-1.93846
C	-2.02899	-1.05835	1.43421
C	-1.74860	-0.06644	2.39602
C	-2.44821	-2.33172	1.86254
C	-1.88999	-0.34082	3.76196
H	-1.40683	0.92031	2.06532
C	-2.57305	-2.61006	3.23230
H	-2.66875	-3.11117	1.12527
C	-2.29637	-1.61741	4.18468
H	-1.66766	0.44174	4.49731
H	-2.89106	-3.60825	3.55652
H	-2.39430	-1.83898	5.25457
C	2.11040	-1.49238	0.85811
C	1.44692	-1.20440	2.06948
C	2.63725	-2.78202	0.65184
C	1.29675	-2.19266	3.04974
H	1.02085	-0.20735	2.22240
C	2.48092	-3.77313	1.63411
H	3.14617	-3.01936	-0.28828
C	1.80579	-3.48347	2.83005
H	0.75482	-1.95966	3.97279
H	2.88200	-4.77867	1.45887
H	1.66931	-4.26424	3.58819
C	3.62637	0.79894	-0.06566
C	3.91229	1.89468	-0.90834
C	4.44775	0.56144	1.05258
C	4.99899	2.73491	-0.63956
H	3.27232	2.08286	-1.78058
C	5.52951	1.41325	1.32772
H	4.23337	-0.28379	1.71532
C	5.80769	2.50082	0.48596
H	5.20983	3.58232	-1.30317
H	6.15957	1.22488	2.20584
H	6.65130	3.16646	0.70425
C	2.58890	-1.08334	-1.96976
C	1.56426	-1.51419	-2.83686
C	3.92992	-1.38634	-2.28217
C	1.87230	-2.25515	-3.98659
H	0.52586	-1.26066	-2.59782
C	4.23633	-2.11808	-3.43914
H	4.73220	-1.04948	-1.61633
C	3.20895	-2.55762	-4.29021
H	1.06472	-2.59353	-4.64623
H	5.28213	-2.34934	-3.67592
H	3.45289	-3.12983	-5.19347
C	-2.16312	3.18853	-0.25523
C	-0.91477	3.00344	-0.90518
C	-2.21374	3.40508	1.11850
H	-0.87519	2.98253	-2.00146
H	-3.17784	3.53687	1.62258
C	0.30881	3.07521	-0.16510
C	-1.02023	3.42606	1.88250
H	1.27003	3.21733	-0.66653
H	-1.06370	3.57933	2.96607
C	0.20952	3.26539	1.24506
H	-3.08561	3.14831	-0.84302
I	1.99225	3.26862	2.38425

E(DMF)= -2729.350916162868; G= 0.56909995

Pd(PPh₃)(CO)(PhI) (**11ad**)

Pd	0.45453	-0.66489	-1.27067
P	-1.44219	0.14117	-0.17051
C	-3.02831	-0.58117	-0.78627
C	-4.23086	0.15119	-0.82957
C	-3.02236	-1.92976	-1.19575
C	-5.41290	-0.46194	-1.27257
H	-4.24143	1.20295	-0.52430
C	-4.20677	-2.54098	-1.62891
H	-2.07692	-2.48646	-1.18355
C	-5.40399	-1.80775	-1.66982
H	-6.34435	0.11626	-1.30984
H	-4.19261	-3.58953	-1.94802
H	-6.32821	-2.28280	-2.01969
C	-1.77613	1.95243	-0.27856
C	-1.81987	2.51601	-1.57127
C	-1.92104	2.78913	0.84174
C	-2.01972	3.89127	-1.73854
H	-1.68914	1.86846	-2.44760
C	-2.10886	4.17044	0.67209
H	-1.87336	2.36349	1.84894
C	-2.16107	4.72472	-0.61513
H	-2.05841	4.31816	-2.74806
H	-2.21608	4.81484	1.55282
H	-2.31197	5.80296	-0.74600
C	-1.50368	-0.22898	1.63503
C	-0.31584	-0.63129	2.27502
C	-2.69323	-0.12764	2.38484
C	-0.30865	-0.90667	3.65011
H	0.59994	-0.74364	1.68436
C	-2.68414	-0.40332	3.75928
H	-3.62819	0.16145	1.89230
C	-1.49180	-0.78972	4.39493
H	0.62338	-1.22328	4.13285
H	-3.61325	-0.32243	4.33662
H	-1.49028	-1.01220	5.46866
C	1.34081	3.05460	-0.31726
C	1.93674	2.16427	-1.22131
C	1.45055	2.82458	1.06153
H	1.85552	2.33416	-2.30136
H	0.97865	3.51280	1.77130
C	2.64547	1.03757	-0.75814
C	2.14330	1.70383	1.54514
H	3.15755	0.37579	-1.46174
H	2.21212	1.51780	2.62168
C	2.73899	0.82135	0.63036
I	3.75945	-0.89013	1.35084
C	1.22405	-2.06938	-2.28197
O	1.56296	-3.01288	-2.86275
H	0.77438	3.91559	-0.68572

E(DMF)= -1806.633386218592; G= 0.31576244

Pd(CO)₂(PhI) (**12ad**)

Pd	-1.36839	-0.16892	0.01411
C	-2.01925	-0.17406	1.82883
O	-2.54029	-0.18729	2.85790
C	-2.05743	-0.31007	-1.78081
O	-2.60127	-0.40082	-2.79402
C	0.74150	3.49394	-0.09355
C	0.89673	2.83838	1.13738
C	1.16017	1.46066	1.18244
C	1.26114	0.74465	-0.02689
C	1.11608	1.39283	-1.26956
C	0.85272	2.77131	-1.29099
H	0.53089	4.56899	-0.11953
H	0.81033	3.39702	2.07660
H	1.28373	0.94787	2.14129
H	1.20696	0.82817	-2.20257
H	0.73147	3.27737	-2.25588

I 1.73095 -1.33041 0.02275
E(DMF)= -883.937973645313; G= 0.06381207

Pd(PPh₃)(PhI) (**13ad**)

Pd	-0.88083	1.58395	1.02500
P	-1.98240	-0.37019	0.74315
C	-1.09969	-1.70174	-0.18359
C	-1.69340	-2.44580	-1.22019
C	0.23361	-1.97436	0.18813
C	-0.96294	-3.45215	-1.87255
H	-2.72603	-2.23785	-1.51763
C	0.95475	-2.98784	-0.45565
H	0.70031	-1.38269	0.98604
C	0.35777	-3.72863	-1.49003
H	-1.43152	-4.02341	-2.68315
H	1.98815	-3.19703	-0.15528
H	0.92467	-4.51695	-1.99957
C	-3.57801	-0.21677	-0.17706
C	-3.62291	0.69475	-1.25236
C	-4.72597	-0.96776	0.13970
C	-4.79270	0.83776	-2.01080
H	-2.73340	1.29695	-1.48050
C	-5.90011	-0.81297	-0.61385
H	-4.70165	-1.67000	0.98004
C	-5.93505	0.08537	-1.69113
H	-4.81680	1.54614	-2.84786
H	-6.79224	-1.39644	-0.35590
H	-6.85430	0.20527	-2.27713
C	-2.47957	-1.23834	2.29793
C	-2.79830	-0.44430	3.41785
C	-2.56557	-2.64080	2.39747
C	-3.21553	-1.04334	4.61448
H	-2.70109	0.64670	3.34352
C	-2.97426	-3.23848	3.59986
H	-2.30963	-3.26598	1.53471
C	-3.30356	-2.44195	4.70774
H	-3.46312	-0.41755	5.48033
H	-3.03512	-4.33160	3.67106
H	-3.62230	-2.91077	5.64656
C	-0.10531	4.69662	-1.40262
C	1.00694	3.91531	-1.04620
C	-1.16362	4.86863	-0.49490
H	1.83000	3.77007	-1.75659
H	-2.03755	5.47016	-0.77332
C	1.08477	3.31472	0.22107
C	-1.11656	4.28093	0.78012
H	1.96620	2.73461	0.51167
H	-1.92210	4.44725	1.50228
C	0.01160	3.49121	1.13809
I	0.33593	2.99446	3.27599
H	-0.14933	5.16767	-2.39110

E(DMF)= -1693.299704245450; G= 0.30701966

Pd(CO)(PhI) (**14ad**)

Pd	0.86157	1.50838	1.14007
C	-1.99161	4.04264	0.24518
C	-0.68655	4.54779	0.13030
C	-2.30274	3.12433	1.26069
H	-0.43577	5.25361	-0.67062
H	-3.31703	2.71703	1.34465
C	0.31293	4.16738	1.04109
C	-1.32780	2.72220	2.18881
H	1.31773	4.59656	0.97865
H	-1.58442	2.04321	3.00794

C	-0.01033	3.25298	2.08442
I	1.37157	3.00080	3.74228
C	1.51310	0.02020	0.19198
O	1.92217	-0.89494	-0.38394
H	-2.76562	4.35840	-0.46307

E(DMF)= -770.625389448368; G= 0.05780063

[Pd(PPh₃)₂(CO)(PhI)][‡] (**7TS**)

Pd	0.25151	0.95088	-0.58231
P	-1.57490	-0.46444	0.04569
P	2.17095	-0.55443	-0.39548
C	-1.44790	-2.03926	-0.90787
C	-1.99477	-2.13651	-2.20690
C	-0.63952	-3.08893	-0.42644
C	-1.72964	-3.26021	-3.00349
H	-2.62209	-1.32848	-2.59696
C	-0.37963	-4.20863	-1.22677
H	-0.20433	-3.02987	0.57383
C	-0.91676	-4.29782	-2.51944
H	-2.16048	-3.32091	-4.00968
H	0.26390	-5.00690	-0.83842
H	-0.69959	-5.16862	-3.14902
C	-3.22745	0.19188	-0.46783
C	-3.27915	1.04395	-1.58728
C	-4.41773	-0.12080	0.20914
C	-4.49959	1.55321	-2.04197
H	-2.34856	1.32761	-2.08712
C	-5.64500	0.40037	-0.23267
H	-4.38957	-0.76220	1.09436
C	-5.68811	1.23486	-1.36293
H	-4.51873	2.21853	-2.91875
H	-6.56550	0.16624	0.31581
H	-6.64381	1.64552	-1.70694
C	-1.86485	-1.03364	1.77732
C	-1.47302	-0.17579	2.82319
C	-2.46737	-2.26798	2.09233
C	-1.67803	-0.54270	4.15999
H	-0.97507	0.77390	2.59009
C	-2.66604	-2.63659	3.43001
H	-2.77474	-2.94520	1.28887
C	-2.27811	-1.77263	4.46747
H	-1.36947	0.13832	4.96142
H	-3.11796	-3.60707	3.66421
H	-2.43242	-2.06647	5.51207
C	2.15947	-1.86001	0.89980
C	1.53287	-1.54878	2.12734
C	2.63398	-3.16630	0.67785
C	1.37072	-2.53368	3.10748
H	1.15055	-0.53878	2.29163
C	2.46812	-4.14882	1.66462
H	3.10941	-3.41924	-0.27468
C	1.83189	-3.83873	2.87589
H	0.85602	-2.28340	4.04306
H	2.83641	-5.16567	1.48106
H	1.69139	-4.61341	3.63805
C	3.65825	0.45542	-0.01383
C	3.99279	1.47710	-0.93062
C	4.40451	0.32085	1.16999
C	5.06671	2.33537	-0.67327
H	3.39623	1.60118	-1.84249
C	5.47919	1.19114	1.42934
H	4.14997	-0.46411	1.89028
C	5.81454	2.19574	0.51079
H	5.31578	3.12409	-1.39449
H	6.05618	1.07900	2.35621
H	6.65219	2.87429	0.71487
C	2.66821	-1.45224	-1.92336
C	1.66523	-1.84730	-2.83041
C	4.01788	-1.76424	-2.19972

C	2.00430	-2.55224	-3.99475
H	0.61803	-1.60074	-2.62398
C	4.35136	-2.46460	-3.36782
H	4.79923	-1.45387	-1.50078
C	3.34318	-2.85947	-4.26692
H	1.21382	-2.86214	-4.68713
H	5.40231	-2.70498	-3.57677
H	3.60839	-3.40347	-5.18171
C	0.39724	1.41257	-2.46712
O	0.44792	1.53227	-3.61814
C	-2.91544	4.72490	-0.76460
C	-1.64250	4.84395	-1.34809
C	-3.10974	3.79849	0.26834
H	-1.46844	5.56906	-2.14905
H	-4.09200	3.69629	0.74853
C	-0.57807	4.03790	-0.92080
C	-2.05459	2.98237	0.70875
H	0.41400	4.13521	-1.38783
H	-2.22410	2.28594	1.53612
C	-0.80301	3.06966	0.08004
I	1.10305	2.68141	1.52800
H	-3.74045	5.35863	-1.10388

E(DMF)= -2842.615010000049; G= 0.56210433

[Pd(PPh₃)(CO)₂(PhI)][‡] (**8TS**)

Pd	-0.93079	0.79174	-0.00440
P	1.42796	0.06221	0.06545
C	1.83366	-1.32330	-1.06458
C	2.51676	-2.47894	-0.64036
C	1.40343	-1.22329	-2.40510
C	2.77841	-3.51444	-1.55125
H	2.84553	-2.56731	0.40023
C	1.67902	-2.25288	-3.31298
H	0.84406	-0.33880	-2.73082
C	2.36586	-3.40238	-2.88724
H	3.30926	-4.41220	-1.21263
H	1.34190	-2.16550	-4.35239
H	2.57180	-4.21342	-3.59582
C	1.96755	-0.52537	1.71960
C	3.19949	-0.15645	2.29267
C	1.09287	-1.37177	2.43391
C	3.55189	-0.63012	3.56568
H	3.88158	0.50196	1.74438
C	1.45503	-1.84997	3.69921
H	0.12697	-1.64808	1.99477
C	2.68381	-1.47789	4.26970
H	4.51047	-0.33384	4.00740
H	0.76957	-2.50727	4.24740
H	2.96040	-1.84384	5.26496
C	2.64140	1.36988	-0.36454
C	3.79447	1.11477	-1.13242
C	2.39553	2.67635	0.10743
C	4.69129	2.15487	-1.41888
H	3.98682	0.10329	-1.50510
C	3.29977	3.70933	-0.17227
H	1.48713	2.87979	0.68709
C	4.44857	3.45091	-0.93795
H	5.58598	1.94975	-2.01889
H	3.10236	4.72119	0.20029
H	5.15152	4.26126	-1.16488
C	-0.76399	1.97385	-1.58174
O	-0.47398	2.67429	-2.45208
C	-1.04179	1.33507	1.88761
O	-0.92494	1.64395	2.99337
C	-5.80453	1.53339	-0.13516
C	-5.10317	1.46511	-1.35010
C	-3.84632	0.84285	-1.41808
C	-3.28058	0.31658	-0.24497
C	-3.98841	0.33353	0.96826

C	-5.24416	0.95977	1.01756
H	-6.78821	2.01361	-0.09139
H	-5.53465	1.89263	-2.26359
H	-3.31608	0.77311	-2.37309
H	-3.56699	-0.12805	1.86642
H	-5.78672	0.98930	1.97088
I	-1.97418	-1.76438	-0.62065

E(DMF)= -1919.910072178766; G= 0.31236825

[Pd(CO)₃(PhI)][‡] (**9TS**)

Pd	-0.79640	1.11691	0.05924
C	-0.65274	2.61167	-1.28385
O	-0.53611	3.50353	-1.99776
C	-0.71581	1.55563	2.02490
O	-0.60216	1.83054	3.13408
C	-5.41256	2.94712	0.12285
C	-4.79532	2.69009	-1.11123
C	-3.67745	1.84290	-1.19031
C	-3.16563	1.28617	-0.00876
C	-3.79085	1.49629	1.22841
C	-4.91057	2.34284	1.28589
H	-5.18596	3.13967	-2.03192
H	-3.22213	1.62158	-2.16007
H	-3.42618	1.00771	2.13645
H	-5.39381	2.51735	2.25486
I	-2.42348	-1.14184	-0.36045
C	0.94659	0.04245	-0.25366
O	1.85803	-0.64306	-0.35942
H	-6.29212	3.59857	0.17536

E(DMF)= -997.229131449023; G= 0.06271874

[Pd(PPh₃)₂(PhI)][‡] (**10TS**)

Pd	0.20213	0.90518	0.04767
P	-1.66429	-0.48888	0.20146
P	2.18984	-0.27901	-0.30859
C	-1.51993	-2.09172	-0.71216
C	-2.12136	-2.29658	-1.97053
C	-0.65481	-3.08511	-0.20285
C	-1.85110	-3.45994	-2.70770
H	-2.80255	-1.54417	-2.38085
C	-0.39232	-4.24608	-0.93956
H	-0.18147	-2.94939	0.77276
C	-0.98259	-4.43693	-2.19867
H	-2.32591	-3.60042	-3.68621
H	0.28949	-4.99930	-0.52820
H	-0.76658	-5.34109	-2.78014
C	-3.26635	0.17665	-0.42422
C	-3.23545	0.86956	-1.65198
C	-4.48637	0.06087	0.26800
C	-4.41063	1.39509	-2.20183
H	-2.27417	1.02103	-2.15805
C	-5.65826	0.61370	-0.27128
H	-4.52061	-0.45801	1.23133
C	-5.62666	1.27002	-1.51139
H	-4.37105	1.92918	-3.15783
H	-6.60316	0.52490	0.27880
H	-6.54576	1.69454	-1.93233
C	-2.05838	-1.05265	1.91710
C	-1.65694	-0.23763	2.99377
C	-2.72483	-2.26547	2.18534
C	-1.91540	-0.62685	4.31602
H	-1.11944	0.69585	2.79053
C	-2.97483	-2.65807	3.50801
H	-3.03988	-2.90771	1.35591

C	-2.57023	-1.84094	4.57618
H	-1.59437	0.01675	5.14350
H	-3.48641	-3.60760	3.70634
H	-2.76475	-2.15187	5.60971
C	2.21875	-1.71850	0.85394
C	1.65575	-1.52853	2.13377
C	2.69745	-2.99143	0.49484
C	1.55156	-2.59905	3.03052
H	1.26281	-0.54261	2.40434
C	2.59461	-4.06304	1.39590
H	3.12713	-3.15166	-0.49904
C	2.01454	-3.87313	2.65953
H	1.08556	-2.44190	4.00983
H	2.96031	-5.05466	1.10323
H	1.91992	-4.71674	3.35396
C	3.77784	0.58044	0.07344
C	3.98092	1.85274	-0.49947
C	4.76345	0.04481	0.92449
C	5.15695	2.56805	-0.24348
H	3.20040	2.28256	-1.14019
C	5.93655	0.76924	1.19029
H	4.61458	-0.94020	1.37904
C	6.13779	2.02814	0.60582
H	5.30259	3.55655	-0.69423
H	6.69785	0.34571	1.85711
H	7.05312	2.59377	0.81769
C	2.52893	-1.06953	-1.93906
C	1.41994	-1.48706	-2.70237
C	3.83138	-1.30137	-2.42514
C	1.61033	-2.14692	-3.92358
H	0.40894	-1.29682	-2.32845
C	4.01770	-1.95126	-3.65476
H	4.69715	-0.97667	-1.83762
C	2.90938	-2.37908	-4.40340
H	0.73836	-2.47722	-4.49953
H	5.03388	-2.12765	-4.02811
H	3.05914	-2.88742	-5.36323
C	-2.52971	4.22324	-1.43738
C	-1.18286	4.11944	-1.80399
C	-2.95372	3.73624	-0.18396
H	-0.83918	4.50825	-2.77028
H	-4.01239	3.78800	0.09543
C	-0.24401	3.54639	-0.92379
C	-2.04498	3.15078	0.69837
H	0.81976	3.52138	-1.18233
H	-2.37968	2.76200	1.66478
C	-0.69094	3.02186	0.31181
I	0.88584	2.91390	1.96567
H	-3.25474	4.67996	-2.12031

E(DMF)= -2729.306154068945; G= 0.55982632

[Pd(PPh₃)(CO)(PhI)][‡] (**11TS**)

Pd	0.40968	1.25051	0.50373
P	-1.32544	-0.39111	0.42776
C	-0.81002	-2.02855	-0.24721
C	-1.47902	-2.67783	-1.30217
C	0.31738	-2.64289	0.33779
C	-1.02337	-3.92273	-1.76512
H	-2.35656	-2.21293	-1.76313
C	0.76269	-3.88858	-0.12031
H	0.84565	-2.13823	1.15573
C	0.09483	-4.53120	-1.17658
H	-1.54905	-4.41898	-2.58970
H	1.64026	-4.35556	0.34152
H	0.44797	-5.50265	-1.54035
C	-2.74563	0.08130	-0.63979
C	-2.43749	0.57000	-1.92690
C	-4.08888	0.03623	-0.22373
C	-3.45815	0.98493	-2.78932

H	-1.38905	0.63970	-2.24118
C	-5.10892	0.46571	-1.08686
H	-4.33953	-0.32520	0.77845
C	-4.79790	0.93723	-2.37044
H	-3.20538	1.36571	-3.78549
H	-6.15269	0.43341	-0.75082
H	-5.59633	1.27501	-3.04152
C	-2.08398	-0.88239	2.03681
C	-1.86086	-0.08092	3.17273
C	-2.86602	-2.05046	2.15517
C	-2.43301	-0.42814	4.40609
H	-1.22060	0.80533	3.09297
C	-3.43484	-2.39527	3.38877
H	-3.01988	-2.69338	1.28073
C	-3.22313	-1.58207	4.51494
H	-2.25066	0.20192	5.28468
H	-4.03924	-3.30636	3.47434
H	-3.66632	-1.85552	5.47965
C	-2.88439	3.94236	-1.14532
C	-1.52488	4.06755	-1.45000
C	-3.27410	3.36502	0.07990
H	-1.20642	4.54170	-2.38642
H	-4.33800	3.25456	0.31992
C	-0.54409	3.62649	-0.53988
C	-2.32149	2.89797	0.98565
H	0.51757	3.80618	-0.74270
H	-2.63373	2.43311	1.92550
C	-0.95025	2.98284	0.65302
I	0.56476	3.23597	2.45876
C	2.06448	0.39979	-0.05712
O	2.96079	-0.22834	-0.42786
H	-3.64406	4.30030	-1.84827

E(DMF)= -1806.618934404858; G= 0.30808857

[Pd(CO)₂(PhI)][‡] (**12TS**)

Pd	-1.64860	0.40305	-0.34861
C	-0.12088	0.52462	-1.62291
O	0.77012	0.56806	-2.34637
C	-1.25403	1.19214	1.42881
O	-0.90947	1.61819	2.43925
C	-5.97770	1.96309	0.50777
C	-5.37918	2.04070	-0.75523
C	-4.30424	1.19263	-1.08822
C	-3.80660	0.31328	-0.10930
C	-4.42411	0.19421	1.14964
C	-5.50081	1.03394	1.45375
H	-6.82887	2.60833	0.75375
H	-5.76195	2.73818	-1.51029
H	-3.87768	1.21345	-2.09694
H	-4.04755	-0.52247	1.88653
H	-5.96758	0.96875	2.44415
I	-2.97575	-1.84030	-1.11403

E(DMF)= -883.925068972364; G= 0.06085995

[Pd(PPh₃)(PhI)][‡] (**13TS**)

Pd	-0.24806	1.44446	0.79962
P	-1.39925	-0.49405	0.58183
C	-0.81125	-2.03803	-0.23912
C	-1.62785	-2.80930	-1.08995
C	0.50325	-2.46692	0.03394
C	-1.13599	-3.99754	-1.65066
H	-2.64847	-2.47967	-1.31112
C	0.98851	-3.65930	-0.52046
H	1.14230	-1.85298	0.68162

C	0.16935	-4.42693	-1.36402
H	-1.77742	-4.59342	-2.31165
H	2.01113	-3.98647	-0.29941
H	0.54970	-5.35741	-1.80124
C	-2.86026	-0.01452	-0.44989
C	-2.61153	0.46088	-1.75530
C	-4.18062	-0.02418	0.03632
C	-3.66567	0.89911	-2.56422
H	-1.58074	0.50109	-2.12804
C	-5.23384	0.43673	-0.77129
H	-4.38813	-0.38562	1.04867
C	-4.98220	0.89379	-2.07278
H	-3.45710	1.26281	-3.57706
H	-6.25863	0.43108	-0.37942
H	-5.80679	1.24948	-2.70167
C	-2.18501	-1.12304	2.13179
C	-2.37286	-0.20750	3.18754
C	-2.63223	-2.45001	2.28039
C	-3.01740	-0.60763	4.36614
H	-1.99785	0.81771	3.07416
C	-3.26601	-2.85112	3.46668
H	-2.48379	-3.17081	1.46882
C	-3.46392	-1.93149	4.50862
H	-3.16237	0.11326	5.17980
H	-3.60884	-3.88706	3.57583
H	-3.95934	-2.24814	5.43420
C	-2.41543	3.99698	-1.56187
C	-1.02334	4.05779	-1.71359
C	-2.97461	3.71782	-0.30194
H	-0.58271	4.28175	-2.69266
H	-4.06273	3.64989	-0.18630
C	-0.17116	3.83627	-0.61631
C	-2.15393	3.49425	0.80973
H	0.91543	3.90912	-0.72870
H	-2.58707	3.28221	1.79171
C	-0.74309	3.51728	0.64023
I	0.54928	3.60243	2.45745
H	-3.06967	4.16375	-2.42438

E(DMF)= -1693.294094080908; G= 0.30511034

[Pd(CO)(PhI)][‡] (14TS)

Pd	0.35607	1.72386	0.38146
C	-2.66147	3.56321	-1.26966
C	-1.41976	4.19836	-1.42955
C	-2.95583	2.88371	-0.07701
H	-1.18118	4.71659	-2.36552
H	-3.91868	2.37441	0.04506
C	-0.47013	4.18938	-0.39427
C	-2.03001	2.85466	0.97946
H	0.47954	4.72241	-0.50236
H	-2.27880	2.36531	1.92611
C	-0.78008	3.51968	0.82388
I	0.46540	3.85935	2.56891
C	1.22747	0.14309	-0.14451
O	1.76053	-0.83043	-0.46798
H	-3.39764	3.58941	-2.08116

E(DMF)= -770.609616288554; G= 0.05695483

Pd(PPh₃)₂(CO)(Ph)(I) (7II)

Pd	-0.63989	-0.92524	0.67071
P	-0.61989	1.64179	0.63229
P	1.53855	-1.29210	-0.37170
H	-1.92526	4.48921	-4.19883
H	3.12530	2.70482	-4.18248

H	0.75429	1.88313	-4.09683
H	2.74036	-4.45158	-4.06704
H	-2.69656	2.12744	-3.84702
C	2.83973	1.91554	-3.47626
C	1.51394	1.45413	-3.43405
C	-1.67233	3.95754	-3.27350
C	-2.10693	2.63848	-3.07658
C	2.29603	-4.34178	-3.07119
H	2.60244	-2.19404	-3.01459
H	1.86050	-6.45670	-2.85592
H	4.83631	1.71990	-2.64207
C	3.79876	1.36613	-2.61055
C	1.14472	0.45752	-2.52180
H	0.11503	0.08807	-2.48901
C	2.21808	-3.06987	-2.48252
H	-0.57472	5.63048	-2.42602
C	1.80236	-5.46474	-2.39208
C	-0.91226	4.59758	-2.28028
C	-1.77573	1.95583	-1.89728
H	-2.08616	0.91173	-1.77055
C	3.43103	0.37850	-1.68530
C	2.09731	-0.07249	-1.62964
I	-1.81875	-1.91407	-1.65474
C	1.63571	-2.92042	-1.21186
C	1.22233	-5.31598	-1.12113
C	-0.58555	3.92102	-1.09710
H	4.17421	-0.02203	-0.98908
C	-1.00899	2.58974	-0.90053
H	1.81495	2.49379	-0.80155
H	0.82343	-6.18900	-0.59212
C	1.13113	-4.04867	-0.53535
H	0.00158	4.42816	-0.32421
H	3.91372	-3.10365	-0.07821
H	-3.30691	0.61429	0.03410
H	4.04085	3.26667	-0.04725
C	1.99681	2.64421	0.26454
H	0.64778	-3.92656	0.44036
H	-2.60580	3.90714	0.63648
C	3.97084	-2.33757	0.70213
C	3.25364	3.08850	0.69423
C	2.96132	-1.35957	0.80253
C	-3.55541	-0.03412	0.87618
H	-5.55821	0.76644	0.99941
C	0.96724	2.39751	1.19709
C	-4.84325	0.05065	1.42356
H	5.82758	-3.09841	1.51807
C	-2.60403	-0.92519	1.40419
C	5.04844	-2.33050	1.60081
C	-2.68032	3.37875	1.59210
C	-1.83395	2.28865	1.86476
C	3.04537	-0.38250	1.81325
H	2.26365	0.37578	1.90440
C	3.50437	3.29607	2.05894
H	-4.29998	4.62649	2.30823
C	0.02305	-1.61634	2.34426
H	4.48996	3.63880	2.39440
C	-3.64038	3.77989	2.53430
C	-5.21274	-0.76687	2.50166
C	-2.99216	-1.77186	2.45777
C	5.13097	-1.34847	2.60002
C	1.22214	2.61869	2.56685
C	4.12658	-0.37345	2.70278
H	-6.21703	-0.69452	2.93587
H	-2.30132	-2.51203	2.87368
C	2.48190	3.06483	2.99179
C	-4.28531	-1.68634	3.00700
C	-1.96538	1.60805	3.09354
H	5.97555	-1.34641	3.29999
O	0.43630	-1.92167	3.37862
H	0.43327	2.44791	3.30574
H	-1.34938	0.72628	3.29350
H	4.17670	0.39978	3.47819
C	-3.76266	3.10015	3.75478

H	-4.55791	-2.34813	3.83944
C	-2.91721	2.01496	4.03466
H	2.66146	3.23614	4.06008
H	-4.52178	3.40763	4.48395
H	-3.01705	1.46266	4.97578

E(DMF)= -2842.640032024556; G= 0.56513802

Pd(PPh₃)(CO)₂(Ph)(I) (**8II**)

Pd	-1.03295	0.35535	-0.03268
P	1.30824	-0.22444	0.03107
C	1.88970	-1.62144	-0.99718
C	3.01359	-2.37598	-0.60804
C	1.23345	-1.91423	-2.20759
C	3.48295	-3.40695	-1.43454
H	3.51741	-2.16271	0.34089
C	1.71033	-2.94154	-3.03083
H	0.33361	-1.36093	-2.49116
C	2.83421	-3.68898	-2.64611
H	4.35643	-3.99415	-1.12747
H	1.18884	-3.17113	-3.96667
H	3.19756	-4.50117	-3.28692
C	1.93231	-0.58722	1.71950
C	2.93907	0.19097	2.32332
C	1.36799	-1.67516	2.41908
C	3.37590	-0.11833	3.62063
H	3.38352	1.03395	1.78448
C	1.81348	-1.97713	3.71152
H	0.57603	-2.27266	1.94862
C	2.81623	-1.20054	4.31562
H	4.15969	0.49010	4.08731
H	1.37035	-2.82285	4.24983
H	3.15989	-1.43870	5.32869
C	2.30751	1.21640	-0.52611
C	3.48677	1.05969	-1.27944
C	1.88212	2.51013	-0.16031
C	4.23212	2.18646	-1.65781
H	3.81945	0.05906	-1.57334
C	2.63590	3.63116	-0.53138
H	0.95220	2.63137	0.40797
C	3.81164	3.47128	-1.28278
H	5.14671	2.05706	-2.24819
H	2.30068	4.63325	-0.24001
H	4.39640	4.34908	-1.58101
C	-1.00440	0.95774	-1.85721
O	-1.03576	1.27150	-2.96427
C	-1.18382	0.54423	1.91464
O	-1.35575	0.54300	3.04936
C	-5.56752	2.25713	-0.11802
C	-4.45709	3.06425	0.16862
C	-3.16534	2.50802	0.18360
C	-2.99733	1.13943	-0.07820
C	-4.09826	0.32550	-0.37158
C	-5.38502	0.89288	-0.38950
H	-6.57446	2.69175	-0.13138
H	-4.58968	4.13194	0.38403
H	-2.30179	3.14661	0.40270
H	-3.95933	-0.74215	-0.57299
H	-6.24805	0.25540	-0.61790
I	-1.69703	-2.48808	0.09810

E(DMF)= -1919.953137935720; G= 0.31452974

Pd(CO)₃(Ph)(I) (**9II**)

Pd	-0.92191	0.69586	-0.03598
C	-0.95976	1.38835	-1.88296

O	-1.07822	1.66969	-2.98667
C	-1.18154	0.86046	1.90989
O	-1.42560	0.83457	3.02860
C	-5.59745	2.13162	-0.11135
C	-4.57177	3.06525	0.09374
C	-3.22901	2.64652	0.11358
C	-2.93387	1.28817	-0.07257
C	-3.94511	0.34312	-0.27850
C	-5.28319	0.77696	-0.29679
H	-4.80848	4.12583	0.24244
H	-2.43098	3.37971	0.27546
H	-3.70055	-0.71442	-0.42397
H	-6.08004	0.04100	-0.45871
I	-1.14165	-2.18155	-0.47732
H	-6.64331	2.46040	-0.12702
C	0.98876	0.02616	-0.01512
O	2.08375	-0.30497	0.00788

E(DMF)= -997.249981960426; G= 0.06580066

Pd(PPh₃)₂(Ph)(I) (**10II**)

Pd	-0.85842	-0.69547	0.16411
P	-0.54954	1.50983	0.84592
P	1.36480	-1.16955	-0.63375
H	-1.27873	4.67663	-3.90515
H	2.40846	2.16518	-5.20479
H	0.32187	0.78816	-5.03271
H	2.87589	-4.69637	-3.88986
H	-2.09945	2.31128	-3.81525
C	2.24355	1.52098	-4.33292
C	1.07477	0.74957	-4.23636
C	-1.13563	4.07770	-2.99763
C	-1.59774	2.75480	-2.94739
C	2.47791	-4.48597	-2.89007
H	2.41070	-2.34372	-3.21762
H	2.43655	-6.57158	-2.29367
H	4.11771	2.05971	-3.37700
C	3.19977	1.46343	-3.30837
C	0.85322	-0.06010	-3.11580
H	-0.06722	-0.65085	-3.03285
C	2.21701	-3.15869	-2.51275
H	-0.11898	5.66691	-1.91876
C	2.23154	-5.53646	-1.99572
C	-0.48475	4.63414	-1.88404
C	-1.40829	1.98549	-1.79078
H	-1.74488	0.94277	-1.75627
C	2.99019	0.64097	-2.19052
C	1.81062	-0.11910	-2.07964
I	-1.90219	-2.65000	-1.34652
C	1.70172	-2.88114	-1.23565
C	1.71697	-5.25995	-0.71779
C	-0.29784	3.87002	-0.72408
H	3.74320	0.60543	-1.39790
C	-0.75978	2.53814	-0.67006
H	2.00869	2.08654	-0.43048
H	1.51120	-6.07773	-0.01733
C	1.44835	-3.94009	-0.34085
H	0.21545	4.30454	0.14026
H	4.32551	-1.60032	-0.73628
H	-3.61559	0.94769	-0.32808
H	4.25988	2.68364	0.42839
C	2.15218	2.25062	0.64021
H	1.02650	-3.72691	0.64822
H	-2.35348	3.92229	0.89109
C	4.06198	-1.29973	0.28389
C	3.41869	2.59445	1.12574
C	2.71822	-1.02427	0.61047
C	-3.76077	0.29721	0.54157
H	-5.74893	1.07355	0.92119
C	1.05921	2.11684	1.51938

C	-4.97154	0.37221	1.25028
H	6.10046	-1.43029	1.00399
C	-2.74478	-0.57831	0.95768
C	5.05704	-1.21862	1.26688
C	-2.50044	3.35800	1.81700
C	-1.76762	2.18117	2.05203
C	2.38140	-0.72554	1.94299
H	1.33191	-0.54597	2.19945
C	3.61108	2.81417	2.49796
H	-4.01554	4.71312	2.56482
H	4.60416	3.07525	2.88127
C	-3.44296	3.79840	2.75844
C	-5.18566	-0.43547	2.37694
C	-2.97535	-1.40914	2.07031
C	4.71660	-0.88775	2.58893
C	1.25227	2.35815	2.89305
C	3.37612	-0.65406	2.92742
H	-6.12895	-0.37127	2.93283
H	-2.20792	-2.12437	2.39382
C	2.52289	2.70392	3.37633
C	-4.18601	-1.33411	2.77978
C	-1.99135	1.45026	3.23610
H	5.49638	-0.82570	3.35738
H	0.41073	2.28050	3.58839
H	-1.45521	0.51050	3.40294
H	3.10131	-0.40667	3.95855
C	-3.66238	3.06763	3.93498
H	-4.34575	-1.98466	3.64958
C	-2.93257	1.89238	4.17249
H	2.66066	2.89030	4.44816
H	-4.41011	3.40524	4.66260
H	-3.11196	1.30281	5.07873

E(DMF)= -2729.340065769617; G= 0.55950615

Pd(PPh₃)(CO)(Ph)(I) (11II)

Pd	-1.01039	0.45266	0.09837
P	1.34940	-0.14520	0.04118
C	1.91591	-1.57033	-0.97127
C	2.18567	-2.82616	-0.39241
C	2.02233	-1.41390	-2.37064
C	2.55868	-3.90940	-1.20171
H	2.11501	-2.96127	0.69186
C	2.39942	-2.49992	-3.17144
H	1.81147	-0.44421	-2.83036
C	2.66555	-3.75002	-2.59138
H	2.77225	-4.88088	-0.74025
H	2.48096	-2.36591	-4.25666
H	2.95825	-4.59834	-3.22119
C	1.98213	-0.53222	1.73032
C	3.19525	-0.02079	2.22860
C	1.20037	-1.37526	2.54851
C	3.62069	-0.35362	3.52375
H	3.80609	0.64387	1.60894
C	1.63400	-1.71411	3.83701
H	0.24625	-1.76411	2.17386
C	2.84538	-1.20204	4.32799
H	4.56397	0.05427	3.90452
H	1.01855	-2.37097	4.46301
H	3.17972	-1.45914	5.33936
C	2.37135	1.26205	-0.54030
C	3.69828	1.08085	-0.98182
C	1.81767	2.55676	-0.51570
C	4.46155	2.18556	-1.38351
H	4.12899	0.07394	-1.01809
C	2.58581	3.65932	-0.91638
H	0.77704	2.69298	-0.19804
C	3.90755	3.47559	-1.34955
H	5.49122	2.03761	-1.72882

H	2.14542	4.66323	-0.90041
H	4.50481	4.33718	-1.66981
C	-1.09906	0.83442	1.95001
O	-1.20185	1.12948	3.05769
C	-5.73414	1.70615	0.11546
C	-4.75040	2.68667	-0.08102
C	-3.38903	2.33538	-0.08059
C	-3.01449	0.99604	0.10709
C	-3.99379	0.01317	0.31710
C	-5.35403	0.37030	0.31524
H	-6.79562	1.98250	0.11268
H	-5.03971	3.73267	-0.24355
H	-2.62928	3.10761	-0.25022
H	-3.70931	-1.03573	0.46496
H	-6.11695	-0.40343	0.46835
I	-1.26007	0.21568	-2.52033

E(DMF)= -1806.646581324074; G= 0.31263887

Pd(CO)₂(Ph)(I) (12II)

Pd	-1.37630	0.11640	0.02083
C	-1.22722	0.34555	-1.89779
O	-1.13877	0.46858	-3.03038
C	-1.60615	-0.09629	1.93262
O	-1.74052	-0.22586	3.06001
C	-5.61853	2.53062	-0.14236
C	-4.42752	3.21494	0.14341
C	-3.20547	2.52030	0.19347
C	-3.18752	1.13801	-0.04330
C	-4.37301	0.44483	-0.32832
C	-5.59044	1.14798	-0.37745
H	-6.56918	3.07557	-0.18261
H	-4.44313	4.29548	0.33197
H	-2.28039	3.06457	0.41847
H	-4.36147	-0.63551	-0.51656
H	-6.51779	0.60760	-0.60381
I	1.00984	-1.15827	0.08912

E(DMF)= -883.952406269753; G= 0.06365603

Pd(PPh₃)(Ph)(I) (13II)

Pd	-1.07020	-0.45803	-0.17744
P	1.28032	-0.82147	-0.02851
C	1.99382	-2.09943	-1.13714
C	3.17724	-2.79365	-0.81949
C	1.33541	-2.36405	-2.35417
C	3.70427	-3.73052	-1.72026
H	3.68535	-2.60395	0.13281
C	1.86747	-3.29908	-3.25271
H	0.39554	-1.84820	-2.58364
C	3.05259	-3.98187	-2.93798
H	4.62678	-4.26726	-1.46927
H	1.34731	-3.50335	-4.19572
H	3.46406	-4.71772	-3.63941
C	1.91085	-1.27423	1.63985
C	3.09576	-0.73285	2.17599
C	1.17282	-2.21696	2.38561
C	3.54025	-1.13528	3.44457
H	3.66919	0.00302	1.60154
C	1.62521	-2.61789	3.64996
H	0.24521	-2.63049	1.97191
C	2.80767	-2.07812	4.18194
H	4.46322	-0.71107	3.85667
H	1.04708	-3.35090	4.22510
H	3.15516	-2.38950	5.17363

C	2.21468	0.71087	-0.44633
C	3.28065	0.74015	-1.36503
C	1.80034	1.91069	0.17197
C	3.92566	1.95296	-1.65482
H	3.60470	-0.18449	-1.85369
C	2.45156	3.11710	-0.11386
H	0.96385	1.89425	0.88396
C	3.51565	3.14038	-1.03071
H	4.75511	1.96800	-2.37220
H	2.12430	4.04237	0.37420
H	4.02151	4.08530	-1.26049
C	-5.23713	1.75636	-0.43217
C	-4.59307	1.34930	-1.61148
C	-3.46493	0.51332	-1.54862
C	-2.95655	0.13569	-0.29154
C	-3.63192	0.48989	0.89168
C	-4.75949	1.32550	0.81600
H	-6.12982	2.39094	-0.48744
H	-4.97814	1.66842	-2.58774
H	-2.98304	0.16821	-2.47121
H	-3.28008	0.12537	1.86392
H	-5.27579	1.62498	1.73637
I	-2.07408	-2.85017	-0.20321

E(DMF)= -1693.297338468137; G= 0.30618890

Pd(CO)(Ph)(I) (**14II**)

Pd	-1.67231	-0.15344	-0.16365
C	-5.11856	3.02763	0.15078
C	-4.64809	2.64916	-1.11713
C	-3.80002	1.53705	-1.25260
C	-3.38510	0.85377	-0.09398
C	-3.90338	1.18114	1.17308
C	-4.75098	2.29575	1.29148
H	-4.95420	3.20878	-2.00909
H	-3.45946	1.21813	-2.24403
H	-3.64382	0.58644	2.05633
H	-5.13813	2.57882	2.27749
I	-3.31918	-2.14567	-0.54130
C	0.07519	-1.07813	-0.21537
O	1.03965	-1.69803	-0.25822
H	-5.79453	3.88553	0.24812

E(DMF)= -770.609559901513; G= 0.05570912

[Pd(PPh₃)₂(CO)(PhINH₂)][‡] (**7bTS**)

Pd	0.28308	1.00044	-0.56934
P	-1.52613	-0.44572	0.00523
P	2.24076	-0.45379	-0.39472
C	-1.43195	-2.05958	-0.88344
C	-1.93328	-2.18147	-2.19623
C	-0.70707	-3.13438	-0.32699
C	-1.71122	-3.35238	-2.93525
H	-2.49536	-1.35556	-2.64423
C	-0.48786	-4.30206	-1.06980
H	-0.30673	-3.06016	0.68675
C	-0.98543	-4.41653	-2.37635
H	-2.10617	-3.42987	-3.95490
H	0.08679	-5.12132	-0.62235
H	-0.80453	-5.32750	-2.95920
C	-3.16349	0.23152	-0.52944
C	-3.20511	0.99973	-1.71111
C	-4.34357	0.06385	0.21886
C	-4.40404	1.57745	-2.14292
H	-2.28067	1.18395	-2.26690
C	-5.54261	0.65258	-0.21139

H	-4.32717	-0.50863	1.15155
C	-5.57695	1.40883	-1.39190
H	-4.41393	2.19570	-3.04698
H	-6.45333	0.52356	0.38641
H	-6.50997	1.88358	-1.71714
C	-1.82480	-0.94857	1.75795
C	-1.34016	-0.10729	2.77831
C	-2.51279	-2.12753	2.11114
C	-1.54305	-0.43181	4.12696
H	-0.77419	0.79265	2.51260
C	-2.70235	-2.45924	3.46027
H	-2.89340	-2.79162	1.32812
C	-2.22061	-1.61171	4.47122
H	-1.15653	0.23383	4.90729
H	-3.23002	-3.38367	3.72443
H	-2.37115	-1.87359	5.52560
C	2.14240	-1.81975	0.83297
C	1.58296	-1.51398	2.09055
C	2.51831	-3.14590	0.54747
C	1.37459	-2.52287	3.03810
H	1.28977	-0.48228	2.30806
C	2.31324	-4.15467	1.50092
H	2.94548	-3.39302	-0.42966
C	1.73183	-3.84936	2.74170
H	0.90864	-2.27508	3.99819
H	2.60074	-5.18712	1.26812
H	1.55521	-4.64296	3.47754
C	3.76645	0.45126	0.08867
C	4.03129	1.67593	-0.55985
C	4.65379	-0.01219	1.07822
C	5.18030	2.40992	-0.24174
H	3.32200	2.05423	-1.30601
C	5.79703	0.73405	1.40447
H	4.45436	-0.95902	1.59101
C	6.06536	1.94168	0.74325
H	5.37567	3.36031	-0.75173
H	6.48326	0.36735	2.17785
H	6.95861	2.52355	1.00033
C	2.73519	-1.31791	-1.94235
C	1.71785	-1.90064	-2.72578
C	4.07592	-1.41708	-2.36588
C	2.03736	-2.58245	-3.90660
H	0.67365	-1.81766	-2.41187
C	4.38984	-2.09016	-3.55623
H	4.87280	-0.96777	-1.76407
C	3.37347	-2.67591	-4.32738
H	1.23435	-3.03095	-4.50255
H	5.43521	-2.15744	-3.88208
H	3.62292	-3.19695	-5.25936
C	0.41228	1.32295	-2.51143
O	0.46335	1.09227	-3.64733
C	-3.30088	4.43546	-0.73570
C	-2.07696	4.60431	-1.42672
C	-3.31064	3.58699	0.39160
H	-2.03141	5.27142	-2.29770
H	-4.23949	3.44132	0.95640
C	-0.91999	3.92704	-1.02501
C	-2.16054	2.89069	0.78359
H	0.01735	4.08887	-1.56596
H	-2.21572	2.24385	1.66251
C	-0.97278	3.01522	0.04483
I	1.06794	2.90256	1.40423
N	-4.47304	5.04220	-1.19477
H	-4.33600	5.90926	-1.70888
H	-5.20586	5.13763	-0.49596

E(DMF)= -2897.966476566279; G= 0.57762380

[Pd(PPh₃)₂(CO)(PhIOH)][‡] (**7cTS**)

Pd	0.30551	0.97376	-0.57125
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P	-1.51933	-0.45108	-0.00280
P	2.23146	-0.51142	-0.41739
C	-1.42427	-2.04061	-0.93203
C	-1.95712	-2.14769	-2.23290
C	-0.66262	-3.10986	-0.41476
C	-1.72783	-3.29888	-3.00091
H	-2.54904	-1.32578	-2.64880
C	-0.43571	-4.25683	-1.18644
H	-0.24120	-3.04715	0.59138
C	-0.96364	-4.35634	-2.48248
H	-2.14806	-3.36592	-4.01124
H	0.16856	-5.07169	-0.77101
H	-0.77646	-5.25073	-3.08847
C	-3.14647	0.26089	-0.51937
C	-3.17784	1.05312	-1.68547
C	-4.32540	0.10582	0.23387
C	-4.36662	1.66598	-2.09713
H	-2.25238	1.22394	-2.24470
C	-5.51228	0.73341	-0.17418
H	-4.31632	-0.48705	1.15400
C	-5.53725	1.51387	-1.33892
H	-4.36936	2.29456	-2.99492
H	-6.42088	0.61758	0.42921
H	-6.46057	2.01940	-1.64394
C	-1.82917	-1.00242	1.73291
C	-1.35900	-0.19015	2.78294
C	-2.52037	-2.19128	2.04364
C	-1.58352	-0.55035	4.11906
H	-0.78797	0.71589	2.55147
C	-2.73102	-2.55915	3.38015
H	-2.88867	-2.83373	1.23691
C	-2.26686	-1.73845	4.42094
H	-1.21019	0.09410	4.92324
H	-3.26228	-3.49038	3.61077
H	-2.43535	-2.02760	5.46530
C	2.17276	-1.84097	0.85225
C	1.59250	-1.52367	2.09789
C	2.57082	-3.16724	0.59475
C	1.39537	-2.51844	3.06343
H	1.27126	-0.49566	2.29160
C	2.37080	-4.16197	1.56330
H	3.00929	-3.42709	-0.37389
C	1.77616	-3.84368	2.79475
H	0.91657	-2.26107	4.01453
H	2.67361	-5.19421	1.35004
H	1.60522	-4.62673	3.54309
C	3.72362	0.47111	0.00372
C	4.15759	1.43282	-0.93544
C	4.36081	0.39786	1.25631
C	5.22762	2.28198	-0.63570
H	3.64749	1.51303	-1.90261
C	5.42700	1.26173	1.55761
H	4.02955	-0.33690	1.99758
C	5.86668	2.20009	0.61420
H	5.55992	3.01825	-1.37747
H	5.91633	1.19583	2.53686
H	6.70083	2.87154	0.85035
C	2.71588	-1.40802	-1.94751
C	1.69181	-1.86562	-2.79983
C	4.06115	-1.68079	-2.27176
C	2.00681	-2.59169	-3.95651
H	0.64705	-1.65119	-2.55779
C	4.37239	-2.39911	-3.43512
H	4.86170	-1.33042	-1.61146
C	3.34650	-2.85687	-4.27839
H	1.19917	-2.94396	-4.60801
H	5.42082	-2.60503	-3.68295
H	3.59424	-3.41541	-5.18901
C	0.47180	1.38697	-2.48723
O	0.57524	1.26989	-3.63683
C	-3.20002	4.47229	-0.56896
C	-1.99465	4.65665	-1.27560
C	-3.22528	3.59097	0.52503

H	-1.95376	5.36002	-2.11944
H	-4.15786	3.45577	1.08233
C	-0.83951	3.94860	-0.91321
C	-2.07817	2.86936	0.87590
H	0.09271	4.11540	-1.46102
H	-2.13041	2.19158	1.73097
C	-0.89468	3.00697	0.12901
I	1.15560	2.79217	1.44885
O	-4.35863	5.11713	-0.90334
H	-4.17670	5.70114	-1.65533

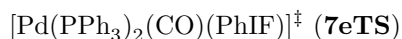
E(DMF)= -2917.845306743885; G= 0.56462648

[Pd(PPh₃)₂(CO)(PhICH₃)][†] (7dTS)

Pd	0.30059	1.00555	-0.57220
P	-1.52022	-0.41921	0.00085
P	2.24875	-0.46093	-0.39509
C	-1.42750	-2.03409	-0.88725
C	-1.92618	-2.15921	-2.20058
C	-0.70699	-3.10893	-0.32530
C	-1.70502	-3.33306	-2.93528
H	-2.48623	-1.33446	-2.65289
C	-0.48847	-4.27935	-1.06393
H	-0.31036	-3.03318	0.68983
C	-0.98268	-4.39672	-2.37140
H	-2.09814	-3.41307	-3.95542
H	0.08253	-5.09874	-0.61219
H	-0.80239	-5.30995	-2.95085
C	-3.15170	0.26299	-0.54391
C	-3.18660	1.00759	-1.74059
C	-4.33553	0.11221	0.20230
C	-4.38494	1.57066	-2.19380
H	-2.25966	1.17985	-2.29600
C	-5.53262	0.68955	-0.24740
H	-4.32358	-0.43993	1.14712
C	-5.56261	1.41571	-1.44702
H	-4.39099	2.15558	-3.12030
H	-6.44635	0.57414	0.34824
H	-6.49760	1.87322	-1.79104
C	-1.82494	-0.92400	1.75148
C	-1.32220	-0.10005	2.77703
C	-2.53426	-2.09272	2.09680
C	-1.52945	-0.43070	4.12363
H	-0.74010	0.79122	2.51722
C	-2.72823	-2.43077	3.44363
H	-2.92720	-2.74409	1.30917
C	-2.22908	-1.59985	4.45996
H	-1.12974	0.22168	4.90842
H	-3.27258	-3.34716	3.70184
H	-2.38325	-1.86649	5.51257
C	2.14819	-1.82390	0.83555
C	1.59567	-1.51358	2.09504
C	2.51475	-3.15255	0.54980
C	1.38499	-2.52024	3.04443
H	1.30984	-0.47992	2.31286
C	2.30719	-4.15913	1.50500
H	2.93632	-3.40348	-0.42879
C	1.73283	-3.84916	2.74784
H	0.92505	-2.26875	4.00644
H	2.58731	-5.19353	1.27195
H	1.55454	-4.64093	3.48519
C	3.77736	0.44195	0.08351
C	4.05601	1.65248	-0.58566
C	4.65220	-0.00759	1.09039
C	5.20588	2.38595	-0.26994
H	3.35703	2.02075	-1.34645
C	5.79658	0.73835	1.41371
H	4.44259	-0.94322	1.61949
C	6.07846	1.93160	0.73259
H	5.41199	3.32515	-0.79623

H	6.47289	0.38252	2.20073
H	6.97259	2.51309	0.98726
C	2.73751	-1.32921	-1.94196
C	1.71529	-1.88372	-2.73894
C	4.08086	-1.46449	-2.34700
C	2.03213	-2.57285	-3.91643
H	0.66974	-1.77340	-2.43802
C	4.39245	-2.14520	-3.53353
H	4.88110	-1.03771	-1.73337
C	3.37076	-2.70220	-4.31897
H	1.22572	-2.99975	-4.52346
H	5.43983	-2.24133	-3.84520
H	3.61860	-3.22952	-5.24785
C	0.43071	1.34705	-2.50888
O	0.46838	1.13571	-3.64882
C	-3.28702	4.44185	-0.70596
C	-2.07177	4.61014	-1.40626
C	-3.28052	3.58945	0.41065
H	-2.03494	5.27984	-2.27612
H	-4.20281	3.43893	0.98512
C	-0.90311	3.94143	-1.02218
C	-2.12439	2.89702	0.80246
H	0.02884	4.10143	-1.57285
H	-2.16763	2.24730	1.67967
C	-0.94409	3.03678	0.05637
I	1.09739	2.91477	1.38121
C	-4.53998	5.15985	-1.14527
H	-4.77908	4.93659	-2.20242
H	-5.40908	4.86051	-0.53515
H	-4.43057	6.25908	-1.06593

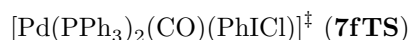
E(DMF)= -2881.913292681420; G= 0.58704964



Pd	0.29562	0.98361	-0.58000
P	-1.52397	-0.44524	-0.01077
P	2.23969	-0.48048	-0.40399
C	-1.42572	-2.05645	-0.90274
C	-1.93486	-2.18609	-2.21128
C	-0.68860	-3.12320	-0.34691
C	-1.70691	-3.35740	-2.94825
H	-2.50827	-1.36727	-2.65782
C	-0.46356	-4.29086	-1.08768
H	-0.28500	-3.04282	0.66527
C	-0.96781	-4.41294	-2.39097
H	-2.10844	-3.44199	-3.96475
H	0.12004	-5.10440	-0.64147
H	-0.78250	-5.32388	-2.97239
C	-3.15179	0.24671	-0.55285
C	-3.18345	0.99680	-1.74661
C	-4.33298	0.11138	0.20060
C	-4.37450	1.58605	-2.18626
H	-2.25762	1.15354	-2.30919
C	-5.52241	0.71458	-0.23587
H	-4.32419	-0.44647	1.14213
C	-5.54807	1.45110	-1.42905
H	-4.37763	2.18073	-3.10660
H	-6.43321	0.61336	0.36684
H	-6.47470	1.93454	-1.75900
C	-1.83240	-0.95662	1.73696
C	-1.33264	-0.13806	2.76811
C	-2.54683	-2.12457	2.07409
C	-1.54951	-0.47191	4.11240
H	-0.74546	0.75171	2.51476
C	-2.75043	-2.46604	3.41861
H	-2.93685	-2.77202	1.28172
C	-2.25554	-1.63951	4.44063
H	-1.15267	0.17665	4.90180
H	-3.29946	-3.38132	3.67059
H	-2.41805	-1.90834	5.49136

C	2.16029	-1.82685	0.84559
C	1.60430	-1.50941	2.10189
C	2.53488	-3.15598	0.57142
C	1.40015	-2.50915	3.06009
H	1.31066	-0.47600	2.31031
C	2.33207	-4.15561	1.53476
H	2.95790	-3.41312	-0.40489
C	1.75571	-3.83842	2.77491
H	0.93813	-2.25230	4.01970
H	2.61757	-5.19039	1.31027
H	1.58133	-4.62493	3.51877
C	3.75206	0.46152	0.04735
C	4.05293	1.60798	-0.71902
C	4.57771	0.12365	1.13552
C	5.17648	2.38557	-0.41788
H	3.39148	1.89174	-1.54659
C	5.69549	0.91595	1.44402
H	4.35085	-0.75988	1.74182
C	6.00055	2.04273	0.66725
H	5.40018	3.27248	-1.02238
H	6.33238	0.64822	2.29601
H	6.87406	2.65971	0.90956
C	2.72939	-1.36121	-1.94238
C	1.70750	-1.88667	-2.75849
C	4.07660	-1.54248	-2.31600
C	2.02794	-2.59204	-3.92576
H	0.65982	-1.74064	-2.48072
C	4.39230	-2.23990	-3.49137
H	4.87581	-1.13859	-1.68568
C	3.37018	-2.76731	-4.29689
H	1.22217	-2.99659	-4.54865
H	5.44252	-2.37310	-3.77865
H	3.62139	-3.30825	-5.21703
C	0.45317	1.35694	-2.50783
O	0.54914	1.18502	-3.65078
C	-3.25988	4.38457	-0.66609
C	-2.07778	4.59091	-1.38989
C	-3.28915	3.54693	0.45065
H	-2.07914	5.26902	-2.25057
H	-4.22313	3.40832	1.00403
C	-0.90888	3.92178	-1.00061
C	-2.12306	2.86433	0.82664
H	0.02125	4.08924	-1.55167
H	-2.15862	2.21054	1.70089
C	-0.94376	3.01220	0.07451
I	1.09997	2.88340	1.38326
F	-4.39277	5.00902	-1.05746

E(DMF)= -2941.870035612938; G= 0.55285243



Pd	0.29264	0.98010	-0.58137
P	-1.52607	-0.44599	-0.01444
P	2.23775	-0.48830	-0.39958
C	-1.42238	-2.05175	-0.91480
C	-1.93329	-2.17603	-2.22308
C	-0.68067	-3.11873	-0.36554
C	-1.70218	-3.34256	-2.96668
H	-2.51056	-1.35688	-2.66398
C	-0.45258	-4.28157	-1.11293
H	-0.27639	-3.04258	0.64670
C	-0.95837	-4.39833	-2.41615
H	-2.10503	-3.42314	-3.98296
H	0.13432	-5.09569	-0.67211
H	-0.77065	-5.30545	-3.00272
C	-3.15432	0.24934	-0.54749
C	-3.18992	1.00453	-1.73820
C	-4.32991	0.12157	0.21599
C	-4.37774	1.61062	-2.16205
H	-2.26835	1.15555	-2.30895

C	-5.51641	0.74132	-0.20561
H	-4.31824	-0.44053	1.15499
C	-5.54467	1.48662	-1.39301
H	-4.38210	2.21768	-3.07381
H	-6.42194	0.64857	0.40636
H	-6.46538	1.99103	-1.70661
C	-1.83019	-0.96608	1.73126
C	-1.33652	-0.14915	2.76656
C	-2.53981	-2.13867	2.06235
C	-1.55413	-0.48968	4.10910
H	-0.75392	0.74492	2.51776
C	-2.74403	-2.48675	3.40504
H	-2.92632	-2.78416	1.26668
C	-2.25489	-1.66213	4.43131
H	-1.16228	0.15752	4.90211
H	-3.28936	-3.40556	3.65215
H	-2.41803	-1.93607	5.48061
C	2.16356	-1.83142	0.85433
C	1.60508	-1.51311	2.10936
C	2.53939	-3.16091	0.58270
C	1.40040	-2.51173	3.06872
H	1.30916	-0.47998	2.31595
C	2.33554	-4.15945	1.54692
H	2.96393	-3.41937	-0.39258
C	1.75715	-3.84111	2.78584
H	0.93655	-2.25410	4.02721
H	2.62164	-5.19441	1.32402
H	1.58175	-4.62688	3.53026
C	3.74618	0.46298	0.04587
C	4.05136	1.59781	-0.73584
C	4.56358	0.14367	1.14573
C	5.17092	2.38225	-0.43738
H	3.39683	1.86679	-1.57372
C	5.67738	0.94285	1.45096
H	4.33332	-0.73134	1.76298
C	5.98689	2.05803	0.65965
H	5.39836	3.25977	-1.05411
H	6.30755	0.68870	2.31211
H	6.85754	2.67998	0.89943
C	2.73246	-1.37158	-1.93483
C	1.71440	-1.88449	-2.76326
C	4.08211	-1.57049	-2.29082
C	2.04087	-2.59432	-3.92638
H	0.66525	-1.72603	-2.49814
C	4.40396	-2.27301	-3.46132
H	4.87818	-1.17654	-1.65026
C	3.38536	-2.78736	-4.27981
H	1.23811	-2.98917	-4.55924
H	5.45599	-2.42070	-3.73453
H	3.64147	-3.33252	-5.19611
C	0.43581	1.35070	-2.51090
O	0.46065	1.18206	-3.65791
C	-3.26750	4.38301	-0.68193
C	-2.07787	4.58461	-1.40263
C	-3.28651	3.54595	0.44034
H	-2.06767	5.25567	-2.26823
H	-4.21307	3.39941	1.00286
C	-0.90833	3.92073	-1.01066
C	-2.11954	2.86880	0.81938
H	0.02091	4.08966	-1.56312
H	-2.15502	2.21926	1.69702
C	-0.93872	3.01328	0.06771
I	1.09237	2.89156	1.37157
Cl	-4.74386	5.17280	-1.20309

E(DMF)= -3302.218621129002; G= 0.55130192

[Pd(PPh₃)₂(CO)(PhICF₃)][‡] (**7gTS**)

Pd	0.29745	0.98372	-0.57439
P	-1.52753	-0.43523	-0.00014

P	2.23481	-0.48933	-0.40343
C	-1.42754	-2.04328	-0.89799
C	-1.94054	-2.17050	-2.20516
C	-0.68959	-3.11119	-0.34570
C	-1.71436	-3.34043	-2.94494
H	-2.51638	-1.35168	-2.64827
C	-0.46627	-4.27739	-1.08934
H	-0.28503	-3.03366	0.66625
C	-0.97344	-4.39673	-2.39171
H	-2.11911	-3.42322	-3.96027
H	0.11778	-5.09209	-0.64591
H	-0.78967	-5.30658	-2.97530
C	-3.15266	0.26167	-0.53786
C	-3.18681	1.00115	-1.73828
C	-4.32927	0.14315	0.22588
C	-4.37556	1.59715	-2.17433
H	-2.26404	1.14629	-2.30917
C	-5.51579	0.75497	-0.20651
H	-4.31823	-0.40622	1.17236
C	-5.54353	1.48191	-1.40532
H	-4.38016	2.18885	-3.09534
H	-6.42196	0.67098	0.40564
H	-6.46424	1.98066	-1.72749
C	-1.83186	-0.95195	1.74615
C	-1.32920	-0.13947	2.78058
C	-2.54975	-2.11917	2.07833
C	-1.54550	-0.47912	4.12354
H	-0.74116	0.75069	2.53104
C	-2.75288	-2.46644	3.42137
H	-2.94314	-2.76117	1.28322
C	-2.25429	-1.64640	4.44680
H	-1.14681	0.16477	4.91580
H	-3.30468	-3.38106	3.66953
H	-2.41658	-1.91971	5.49637
C	2.15941	-1.83583	0.84566
C	1.60419	-1.52045	2.10275
C	2.53625	-3.16387	0.56963
C	1.40351	-2.52129	3.06057
H	1.30762	-0.48819	2.31228
C	2.33661	-4.16461	1.53243
H	2.95836	-3.41929	-0.40753
C	1.76148	-3.84949	2.77370
H	0.94221	-2.26621	4.02099
H	2.62365	-5.19865	1.30672
H	1.58971	-4.63701	3.51706
C	3.74522	0.45721	0.04553
C	4.05580	1.59039	-0.73678
C	4.55797	0.13753	1.14883
C	5.17511	2.37357	-0.43470
H	3.40614	1.85912	-1.57856
C	5.67171	0.93553	1.45770
H	4.32467	-0.73640	1.76648
C	5.98572	2.04954	0.66638
H	5.40673	3.24964	-1.05195
H	6.29847	0.68189	2.32137
H	6.85617	2.67072	0.90881
C	2.72065	-1.36494	-1.94523
C	1.69680	-1.87668	-2.76735
C	4.06765	-1.55666	-2.31442
C	2.01513	-2.57855	-3.93736
H	0.64948	-1.72299	-2.49220
C	4.38121	-2.25083	-3.49222
H	4.86807	-1.16321	-1.67902
C	3.35707	-2.76415	-4.30432
H	1.20813	-2.97257	-4.56534
H	5.43113	-2.39248	-3.77634
H	3.60668	-3.30245	-5.22639
C	0.45679	1.37413	-2.49743
O	0.54224	1.22330	-3.64359
C	-3.23492	4.41861	-0.67293
C	-2.02575	4.61071	-1.37504
C	-3.25221	3.56426	0.43919
H	-1.99189	5.28803	-2.23639

H	-4.17897	3.40947	0.99860
C	-0.86396	3.94059	-0.98680
C	-2.09559	2.87725	0.82707
H	0.07111	4.10689	-1.52973
H	-2.14096	2.22065	1.69862
C	-0.90687	3.02298	0.08703
I	1.10207	2.88579	1.38164
C	-4.47142	5.14298	-1.12916
F	-4.34739	6.49156	-1.01376
F	-4.74039	4.90281	-2.44507
F	-5.57589	4.78427	-0.43073

E(DMF)= -3179.700031758820; G= 0.56269617

[Pd(PPh₃)₂(CO)(PhICN)][‡] (**7hTS**)

Pd	0.29637	0.99125	-0.55983
P	-1.53266	-0.42467	-0.01086
P	2.23407	-0.49245	-0.38960
C	-1.42828	-2.03210	-0.90847
C	-1.94115	-2.16216	-2.21534
C	-0.68865	-3.09762	-0.35379
C	-1.71266	-3.33306	-2.95294
H	-2.51914	-1.34567	-2.65983
C	-0.46324	-4.26469	-1.09530
H	-0.28516	-3.01771	0.65845
C	-0.96987	-4.38691	-2.39767
H	-2.11746	-3.41862	-3.96799
H	0.12152	-5.07797	-0.65029
H	-0.78465	-5.29752	-2.97955
C	-3.15484	0.27475	-0.55246
C	-3.18671	1.00850	-1.75682
C	-4.33104	0.16694	0.21343
C	-4.37238	1.61146	-2.19205
H	-2.26538	1.14411	-2.33196
C	-5.51452	0.78507	-0.21948
H	-4.32190	-0.37728	1.16283
C	-5.54004	1.50859	-1.42058
H	-4.37664	2.19767	-3.11744
H	-6.41989	0.71008	0.39499
H	-6.45592	2.01599	-1.74266
C	-1.83666	-0.94324	1.73445
C	-1.32212	-0.14263	2.77210
C	-2.56745	-2.10393	2.06158
C	-1.53991	-0.48694	4.11368
H	-0.72464	0.74216	2.52613
C	-2.77238	-2.45588	3.40306
H	-2.96897	-2.73724	1.26356
C	-2.26221	-1.64723	4.43187
H	-1.13238	0.14786	4.90874
H	-3.33444	-3.36522	3.64739
H	-2.42605	-1.92404	5.48024
C	2.16359	-1.84049	0.85711
C	1.61417	-1.52677	2.11715
C	2.53650	-3.16864	0.57643
C	1.41574	-2.52911	3.07380
H	1.32020	-0.49441	2.33006
C	2.33903	-4.17094	1.53803
H	2.95394	-3.42266	-0.40311
C	1.77014	-3.85732	2.78256
H	0.95940	-2.27519	4.03690
H	2.62324	-5.20501	1.30905
H	1.60039	-4.64605	3.52505
C	3.74273	0.45846	0.05661
C	4.04906	1.59244	-0.72633
C	4.55879	0.14028	1.15799
C	5.16683	2.37860	-0.42611
H	3.39742	1.85943	-1.56708
C	5.67101	0.94121	1.46486
H	4.32917	-0.73462	1.77563
C	5.98036	2.05648	0.67338

H	5.39504	3.25525	-1.04377
H	6.30038	0.68878	2.32695
H	6.84961	2.67990	0.91425
C	2.71737	-1.36081	-1.93611
C	1.69334	-1.86018	-2.76554
C	4.06465	-1.55792	-2.30174
C	2.01183	-2.55471	-3.93999
H	0.64593	-1.70318	-2.49285
C	4.37829	-2.24514	-3.48352
H	4.86504	-1.17372	-1.66066
C	3.35393	-2.74567	-4.30336
H	1.20489	-2.93915	-4.57393
H	5.42831	-2.39121	-3.76490
H	3.60362	-3.27844	-5.22857
C	0.44896	1.38128	-2.48704
O	0.43798	1.23483	-3.63647
C	-3.26171	4.35287	-0.69481
C	-2.04892	4.55852	-1.40212
C	-3.25009	3.52224	0.44925
H	-2.03836	5.21573	-2.27884
H	-4.17426	3.36291	1.01323
C	-0.87521	3.92397	-0.99825
C	-2.08124	2.87211	0.84389
H	0.05561	4.10007	-1.54553
H	-2.10753	2.23365	1.72961
C	-0.89619	3.01835	0.08934
I	1.10162	2.92088	1.36671
C	-4.48353	4.93950	-1.14774
N	-5.49669	5.39042	-1.53023

E(DMF)= -2934.845722701385; G= 0.55899192

[Pd(PPh₃)₂(CO)(PhINO₂)][‡] (**7iTS**)

Pd	0.31492	1.00621	-0.54754
P	-1.52163	-0.40792	-0.01429
P	2.23833	-0.49239	-0.38708
C	-1.42246	-2.01228	-0.91779
C	-1.92848	-2.13104	-2.22843
C	-0.69796	-3.08787	-0.36291
C	-1.70809	-3.30113	-2.96968
H	-2.49535	-1.30635	-2.67215
C	-0.48029	-4.25406	-1.10827
H	-0.30135	-3.01718	0.65272
C	-0.97993	-4.36514	-2.41431
H	-2.10781	-3.37820	-3.98739
H	0.09240	-5.07577	-0.66299
H	-0.80108	-5.27538	-2.99877
C	-3.13483	0.30513	-0.56228
C	-3.15467	1.05018	-1.75949
C	-4.31750	0.19419	0.19377
C	-4.33502	1.66398	-2.19696
H	-2.22883	1.18801	-2.32693
C	-5.49461	0.82068	-0.24186
H	-4.31725	-0.35654	1.13938
C	-5.50844	1.55666	-1.43538
H	-4.32721	2.26605	-3.11230
H	-6.40363	0.74825	0.36696
H	-6.41993	2.07351	-1.75345
C	-1.83133	-0.93348	1.72779
C	-1.30297	-0.15122	2.77232
C	-2.57929	-2.08596	2.04524
C	-1.52488	-0.50424	4.11093
H	-0.69257	0.72650	2.53361
C	-2.78853	-2.44700	3.38362
H	-2.99065	-2.70625	1.24208
C	-2.26513	-1.65582	4.41924
H	-1.10714	0.11686	4.91143
H	-3.36430	-3.34981	3.62008
H	-2.43259	-1.93940	5.46518
C	2.15620	-1.84722	0.85136

C	1.61503	-1.53661	2.11548
C	2.51831	-3.17638	0.56156
C	1.41361	-2.54274	3.06754
H	1.33146	-0.50304	2.33603
C	2.31828	-4.18239	1.51862
H	2.92984	-3.42814	-0.42094
C	1.75723	-3.87169	2.76742
H	0.96408	-2.29090	4.03433
H	2.59442	-5.21707	1.28273
H	1.58551	-4.66323	3.50642
C	3.74979	0.44812	0.07173
C	4.07553	1.57592	-0.71230
C	4.55000	0.12720	1.18386
C	5.19620	2.35376	-0.40144
H	3.43829	1.84478	-1.56337
C	5.66516	0.91984	1.50095
H	4.30687	-0.74368	1.80195
C	5.99341	2.02936	0.70916
H	5.43981	3.22545	-1.02019
H	6.28213	0.66502	2.37121
H	6.86519	2.64605	0.95792
C	2.72267	-1.35518	-1.93583
C	1.69962	-1.85087	-2.76850
C	4.07052	-1.55570	-2.29734
C	2.01963	-2.54520	-3.94259
H	0.65181	-1.69165	-2.49866
C	4.38563	-2.24276	-3.47877
H	4.87012	-1.17486	-1.65334
C	3.36226	-2.73963	-4.30205
H	1.21349	-2.92693	-4.57914
H	5.43605	-2.39182	-3.75696
H	3.61322	-3.27246	-5.22686
C	0.50340	1.40549	-2.47543
O	0.56257	1.25652	-3.62234
C	-3.25368	4.28318	-0.62660
C	-2.08273	4.50447	-1.37789
C	-3.22438	3.49151	0.53153
H	-2.13180	5.14238	-2.26474
H	-4.14305	3.35003	1.10507
C	-0.88981	3.90105	-0.98789
C	-2.03882	2.86100	0.90380
H	0.02635	4.08408	-1.55699
H	-2.03287	2.23602	1.79924
C	-0.87259	3.00658	0.11376
I	1.13805	2.94618	1.34777
N	-4.52163	4.84853	-1.08083
O	-5.51188	4.70528	-0.35867
O	-4.53871	5.41866	-2.17543

E(DMF)= -3047.121481879091; G= 0.56210340

Pd(PPh₃)₂(CO)(PhINH₂) (**7b**)

Pd	0.29332	1.16566	-0.43049
P	-1.57045	-0.62206	0.12299
P	2.20283	-0.35001	-0.30989
C	-1.41775	-2.20164	-0.82049
C	-1.94431	-2.32987	-2.12326
C	-0.64328	-3.25822	-0.29448
C	-1.68991	-3.48085	-2.88358
H	-2.55956	-1.52998	-2.54631
C	-0.39257	-4.40564	-1.05749
H	-0.23510	-3.18621	0.71548
C	-0.90876	-4.52132	-2.35687
H	-2.10757	-3.56173	-3.89391
H	0.21944	-5.20891	-0.63117
H	-0.70398	-5.41633	-2.95617
C	-3.19832	0.04917	-0.43174
C	-3.24958	0.76318	-1.64789
C	-4.35214	-0.01590	0.37079
C	-4.42636	1.40375	-2.04952

H	-2.34660	0.86705	-2.25578
C	-5.53053	0.63116	-0.03272
H	-4.32709	-0.54905	1.32609
C	-5.56969	1.34697	-1.23717
H	-4.43836	1.97859	-2.98185
H	-6.41906	0.58474	0.60890
H	-6.48247	1.87499	-1.53610
C	-1.91295	-1.19170	1.84318
C	-1.54670	-0.34148	2.90481
C	-2.54383	-2.41985	2.13003
C	-1.79737	-0.71659	4.23248
H	-1.03090	0.60384	2.69805
C	-2.78648	-2.79524	3.45837
H	-2.84669	-3.08318	1.31330
C	-2.41279	-1.94575	4.51309
H	-1.49832	-0.04601	5.04644
H	-3.27382	-3.75415	3.67167
H	-2.60463	-2.24276	5.55126
C	2.09883	-1.76789	0.85603
C	1.48598	-1.56333	2.10772
C	2.58688	-3.04550	0.51876
C	1.33397	-2.63277	2.99966
H	1.12711	-0.56415	2.37379
C	2.44527	-4.10953	1.42120
H	3.05721	-3.21201	-0.45513
C	1.80853	-3.90919	2.65649
H	0.82581	-2.46635	3.95573
H	2.82383	-5.10263	1.15193
H	1.68235	-4.74782	3.35191
C	3.75651	0.51600	0.14330
C	3.99553	1.78960	-0.40923
C	4.71750	-0.07327	0.98372
C	5.19284	2.45963	-0.13311
H	3.22930	2.26217	-1.03483
C	5.91154	0.60781	1.26681
H	4.53249	-1.05984	1.42066
C	6.15208	1.87108	0.70774
H	5.36907	3.45379	-0.55884
H	6.65504	0.14871	1.92950
H	7.08341	2.40361	0.93446
C	2.64317	-1.15713	-1.91104
C	1.62216	-1.78934	-2.64935
C	3.95963	-1.15910	-2.41322
C	1.91359	-2.41766	-3.86604
H	0.59535	-1.78998	-2.27562
C	4.24532	-1.78299	-3.63753
H	4.76167	-0.67083	-1.85076
C	3.22564	-2.41396	-4.36561
H	1.10655	-2.90411	-4.42537
H	5.27190	-1.77229	-4.02357
H	3.45198	-2.89517	-5.32420
C	0.49655	1.30656	-2.33015
O	0.59581	1.34119	-3.48000
C	-3.31121	4.55156	-0.59167
C	-3.19730	3.63858	0.48001
C	-2.29626	4.54040	-1.57029
H	-3.95793	3.63045	1.27188
H	-2.33946	5.25074	-2.40724
C	-2.13521	2.73200	0.54344
C	-1.23334	3.62489	-1.49855
H	-2.09552	2.05234	1.39746
H	-0.47258	3.67008	-2.28519
C	-1.15026	2.68267	-0.45910
I	1.12597	2.31046	1.95330
N	-4.41696	5.40038	-0.70162
H	-4.24773	6.25162	-1.23277
H	-4.88081	5.60589	0.18011

E(DMF)= -2897.991819010305; G= 0.58104681

Pd(PPh₃)₂(CO)(PhIOH) (**7c**)

Pd	0.28988	1.15760	-0.43323
P	-1.56511	-0.60830	0.11504
P	2.19815	-0.35700	-0.31911
C	-1.41319	-2.19227	-0.82168
C	-1.94094	-2.32636	-2.12330
C	-0.64104	-3.24757	-0.29008
C	-1.68956	-3.48202	-2.87744
H	-2.55469	-1.52766	-2.55064
C	-0.39311	-4.39954	-1.04710
H	-0.23305	-3.17134	0.71958
C	-0.91021	-4.52111	-2.34551
H	-2.10822	-3.56771	-3.88695
H	0.21710	-5.20187	-0.61655
H	-0.70776	-5.41980	-2.94004
C	-3.19225	0.05754	-0.44862
C	-3.24125	0.76503	-1.66851
C	-4.35206	-0.01866	0.34405
C	-4.42557	1.38015	-2.08822
H	-2.33392	0.87717	-2.26859
C	-5.53629	0.60689	-0.07510
H	-4.32795	-0.54506	1.30303
C	-5.57634	1.30952	-1.28738
H	-4.43937	1.94184	-3.02879
H	-6.42972	0.55283	0.55872
H	-6.49761	1.81352	-1.60147
C	-1.90927	-1.16949	1.83728
C	-1.54139	-0.31708	2.89655
C	-2.54420	-2.39500	2.12695
C	-1.79505	-0.68728	4.22505
H	-1.02262	0.62623	2.68791
C	-2.78972	-2.76531	3.45612
H	-2.84794	-3.06012	1.31201
C	-2.41472	-1.91355	4.50857
H	-1.49544	-0.01477	5.03714
H	-3.28038	-3.72198	3.67177
H	-2.60923	-2.20645	5.54737
C	2.09788	-1.76885	0.85420
C	1.48848	-1.55932	2.10676
C	2.58520	-3.04766	0.52049
C	1.33853	-2.62542	3.00302
H	1.13088	-0.55907	2.37026
C	2.44556	-4.10826	1.42725
H	3.05305	-3.21811	-0.45393
C	1.81174	-3.90326	2.66326
H	0.83327	-2.45520	3.95998
H	2.82329	-5.10241	1.16078
H	1.68710	-4.73927	3.36208
C	3.75212	0.51298	0.12538
C	3.99963	1.77323	-0.45344
C	4.70306	-0.05897	0.98873
C	5.19478	2.44757	-0.17935
H	3.24158	2.23294	-1.09830
C	5.89521	0.62656	1.26924
H	4.51178	-1.03521	1.44567
C	6.14381	1.87672	0.68508
H	5.37735	3.43173	-0.62518
H	6.63069	0.18133	1.95008
H	7.07335	2.41302	0.91007
C	2.63440	-1.17077	-1.91779
C	1.60849	-1.78449	-2.66449
C	3.95581	-1.20084	-2.40649
C	1.89937	-2.42178	-3.87677
H	0.57845	-1.76475	-2.30034
C	4.24119	-1.83398	-3.62603
H	4.76166	-0.72734	-1.83691
C	3.21619	-2.44608	-4.36286
H	1.08866	-2.89392	-4.44296
H	5.27166	-1.84563	-4.00151
H	3.44249	-2.93470	-5.31771
C	0.49299	1.31547	-2.33426
O	0.57261	1.35761	-3.48552
C	-3.22244	4.62030	-0.52138

C	-3.16630	3.67359	0.51743
C	-2.21135	4.62171	-1.49547
H	-3.94214	3.68254	1.29104
H	-2.22669	5.36803	-2.30311
C	-2.13201	2.73390	0.55456
C	-1.17672	3.66893	-1.44811
H	-2.12005	2.02219	1.38282
H	-0.40717	3.71638	-2.22575
C	-1.13590	2.69297	-0.43930
I	1.14866	2.31121	1.93968
O	-4.26284	5.50723	-0.52841
H	-4.14255	6.10951	-1.27834

E(DMF)= -2917.871918118706; G= 0.56703149

Pd(PPh₃)₂(CO)(PhICH₃) (7d)

Pd	0.29016	1.15320	-0.43499
P	-1.55165	-0.56511	0.09476
P	2.19964	-0.36957	-0.32131
C	-1.40240	-2.15187	-0.83821
C	-1.93232	-2.28690	-2.13879
C	-0.63637	-3.20935	-0.30312
C	-1.68840	-3.44643	-2.88913
H	-2.54143	-1.48573	-2.56811
C	-0.39514	-4.36500	-1.05688
H	-0.22904	-3.13258	0.70677
C	-0.91401	-4.48778	-2.35429
H	-2.10855	-3.53342	-3.89789
H	0.21070	-5.16941	-0.62410
H	-0.71701	-5.38951	-2.94604
C	-3.18449	0.09368	-0.46409
C	-3.24015	0.80389	-1.68185
C	-4.34274	0.00426	0.32929
C	-4.42888	1.41352	-2.09681
H	-2.33315	0.92619	-2.28086
C	-5.53256	0.62116	-0.08677
H	-4.31329	-0.52378	1.28711
C	-5.57886	1.32903	-1.29595
H	-4.44720	1.98098	-3.03371
H	-6.42541	0.55573	0.54686
H	-6.50531	1.82446	-1.60919
C	-1.88539	-1.12808	1.81908
C	-1.49501	-0.29146	2.88236
C	-2.53741	-2.34615	2.10356
C	-1.74395	-0.66948	4.20966
H	-0.96197	0.64506	2.67871
C	-2.77818	-2.72438	3.43128
H	-2.85745	-2.99955	1.28544
C	-2.38112	-1.88783	4.48786
H	-1.42639	-0.00907	5.02480
H	-3.28147	-3.67544	3.64247
H	-2.57135	-2.18681	5.52573
C	2.10162	-1.77220	0.86297
C	1.51224	-1.54559	2.12222
C	2.56602	-3.05997	0.53137
C	1.35659	-2.60414	3.02627
H	1.17525	-0.53743	2.38342
C	2.42192	-4.11285	1.44637
H	3.01813	-3.24411	-0.44795
C	1.80564	-3.89115	2.68832
H	0.86591	-2.42054	3.98830
H	2.78167	-5.11409	1.18151
H	1.67639	-4.72101	3.39357
C	3.75659	0.50087	0.11321
C	4.01675	1.74600	-0.49214
C	4.69633	-0.05563	0.99872
C	5.21230	2.42071	-0.22148
H	3.26833	2.19575	-1.15480
C	5.88926	0.63024	1.27512
H	4.49571	-1.02011	1.47617

C	6.14988	1.86548	0.66531
H	5.40387	3.39369	-0.68766
H	6.61573	0.19708	1.97322
H	7.07971	2.40254	0.88719
C	2.63189	-1.19497	-1.91473
C	1.59718	-1.75756	-2.68831
C	3.96290	-1.28924	-2.36893
C	1.88815	-2.40875	-3.89346
H	0.56034	-1.68697	-2.35066
C	4.24894	-1.93661	-3.58057
H	4.77498	-0.85495	-1.77733
C	3.21446	-2.49818	-4.34436
H	1.07098	-2.84126	-4.48150
H	5.28700	-1.99938	-3.92906
H	3.44161	-2.99827	-5.29310
C	0.59324	1.38384	-2.32209
O	0.73990	1.44986	-3.46571
C	-3.31409	4.53509	-0.53670
C	-3.17668	3.62859	0.53290
C	-2.31340	4.52731	-1.52076
H	-3.92591	3.61732	1.33601
H	-2.37027	5.23514	-2.35925
C	-2.11050	2.72547	0.59121
C	-1.23864	3.61969	-1.46814
H	-2.05381	2.04419	1.44267
H	-0.49083	3.66402	-2.26660
C	-1.14334	2.67931	-0.42965
I	1.19286	2.33598	1.92662
C	-4.50119	5.46453	-0.60947
H	-4.43838	6.14375	-1.47765
H	-5.44553	4.89274	-0.69513
H	-4.58568	6.08718	0.30147

E(DMF)= -2881.937324226219; G= 0.58885242

Pd(PPh₃)₂(CO)(PhIF) (**7e**)

Pd	0.30075	1.16547	-0.44652
P	-1.57051	-0.63946	0.11798
P	2.20579	-0.34882	-0.32427
C	-1.41672	-2.22604	-0.81318
C	-1.94124	-2.36604	-2.11554
C	-0.64155	-3.27706	-0.27693
C	-1.68394	-3.52311	-2.86563
H	-2.55751	-1.57135	-2.54676
C	-0.38854	-4.43070	-1.02958
H	-0.23489	-3.19579	0.73292
C	-0.90241	-4.55798	-2.32879
H	-2.10011	-3.61336	-3.87574
H	0.22322	-5.22981	-0.59527
H	-0.69594	-5.45794	-2.91998
C	-3.19336	0.02990	-0.45422
C	-3.23791	0.72850	-1.67958
C	-4.35463	-0.03209	0.33812
C	-4.41840	1.34648	-2.10632
H	-2.33060	0.82974	-2.28176
C	-5.53470	0.59723	-0.08715
H	-4.33478	-0.55229	1.30061
C	-5.57031	1.28906	-1.30605
H	-4.42851	1.89989	-3.05177
H	-6.42929	0.55271	0.54585
H	-6.48892	1.79389	-1.62649
C	-1.92400	-1.19032	1.84123
C	-1.56772	-0.32530	2.89454
C	-2.55168	-2.41748	2.13903
C	-1.82538	-0.68475	4.22518
H	-1.05482	0.61964	2.67924
C	-2.80127	-2.77698	3.47046
H	-2.84651	-3.09229	1.32875
C	-2.43767	-1.91291	4.51683
H	-1.53482	-0.00285	5.03273

H	-3.28654	-3.73488	3.69273
H	-2.63547	-2.19751	5.55730
C	2.09738	-1.76042	0.84832
C	1.47571	-1.55414	2.09530
C	2.59596	-3.03633	0.51988
C	1.32655	-2.62005	2.99197
H	1.10759	-0.55685	2.35482
C	2.45693	-4.09670	1.42697
H	3.07307	-3.20459	-0.45043
C	1.81240	-3.89461	2.65795
H	0.81215	-2.45227	3.94449
H	2.84387	-5.08840	1.16479
H	1.68881	-4.73052	3.35705
C	3.75762	0.52091	0.12513
C	3.99986	1.78766	-0.44173
C	4.71316	-0.05817	0.97869
C	5.19502	2.46150	-0.16591
H	3.23812	2.25180	-1.07919
C	5.90515	0.62681	1.26098
H	4.52570	-1.03945	1.42639
C	6.14880	1.88337	0.68838
H	5.37410	3.45029	-0.60274
H	6.64453	0.17609	1.93387
H	7.07844	2.41893	0.91460
C	2.64176	-1.16243	-1.92248
C	1.62226	-1.81208	-2.64766
C	3.95456	-1.15400	-2.43403
C	1.91150	-2.44617	-3.86179
H	0.59862	-1.82263	-2.26553
C	4.23780	-1.78409	-3.65575
H	4.75545	-0.65325	-1.88102
C	3.21968	-2.43152	-4.37136
H	1.10583	-2.94604	-4.41118
H	5.26126	-1.76536	-4.04952
H	3.44406	-2.91743	-5.32799
C	0.44480	1.25677	-2.35494
O	0.49772	1.27845	-3.50766
C	-3.18271	4.61259	-0.59753
C	-3.17297	3.67884	0.44280
C	-2.16659	4.63683	-1.55404
H	-3.97100	3.68999	1.19313
H	-2.18517	5.39260	-2.34761
C	-2.13787	2.73641	0.50119
C	-1.13629	3.68103	-1.48148
H	-2.14406	2.02126	1.32629
H	-0.34549	3.72534	-2.23774
C	-1.12262	2.70159	-0.47225
I	1.12124	2.30993	1.92504
F	-4.18921	5.51169	-0.67337

E(DMF)= -2941.895826546393; G= 0.55691824

Pd(PPh₃)₂(CO)(PhICl) (**7f**)

Pd	0.32492	1.18675	-0.43613
P	-1.56459	-0.62452	0.11443
P	2.22200	-0.33789	-0.31329
C	-1.41869	-2.21071	-0.81778
C	-1.94351	-2.34754	-2.12035
C	-0.64894	-3.26568	-0.28154
C	-1.69101	-3.50531	-2.87101
H	-2.55673	-1.55006	-2.55073
C	-0.40091	-4.42012	-1.03465
H	-0.24292	-3.18686	0.72886
C	-0.91442	-4.54406	-2.33435
H	-2.10740	-3.59328	-3.88123
H	0.20642	-5.22259	-0.60026
H	-0.71187	-5.44463	-2.92597
C	-3.18205	0.06260	-0.45158
C	-3.22409	0.75970	-1.67816
C	-4.33364	0.03682	0.35701

C	-4.38715	1.42355	-2.08240
H	-2.32281	0.83345	-2.29364
C	-5.49672	0.71020	-0.04765
H	-4.31625	-0.48330	1.31956
C	-5.52566	1.41075	-1.26143
H	-4.39076	1.98598	-3.02243
H	-6.38108	0.69858	0.60105
H	-6.42367	1.96399	-1.55869
C	-1.92025	-1.17812	1.83653
C	-1.55026	-0.32442	2.89410
C	-2.56572	-2.39735	2.12866
C	-1.81260	-0.68646	4.22313
H	-1.02332	0.61391	2.68406
C	-2.81974	-2.76010	3.45838
H	-2.87120	-3.06337	1.31505
C	-2.44303	-1.90680	4.50897
H	-1.51162	-0.01291	5.03385
H	-3.31876	-3.71196	3.67605
H	-2.64458	-2.19363	5.54807
C	2.09980	-1.75306	0.85333
C	1.48265	-1.54538	2.10218
C	2.58686	-3.03215	0.51980
C	1.32642	-2.61278	2.99587
H	1.12406	-0.54563	2.36534
C	2.44147	-4.09394	1.42417
H	3.06042	-3.20150	-0.45201
C	1.80131	-3.89020	2.65714
H	0.81524	-2.44377	3.94987
H	2.81986	-5.08792	1.15820
H	1.67249	-4.72699	3.35420
C	3.78044	0.51622	0.14158
C	4.03000	1.78861	-0.40925
C	4.73613	-0.08255	0.98154
C	5.23274	2.44831	-0.13177
H	3.26844	2.26812	-1.03540
C	5.93567	0.58817	1.26552
H	4.54281	-1.06824	1.41677
C	6.18674	1.85023	0.70829
H	5.41778	3.44137	-0.55620
H	6.67534	0.12189	1.92736
H	7.12255	2.37437	0.93570
C	2.65112	-1.14933	-1.91427
C	1.62774	-1.79674	-2.63625
C	3.96133	-1.13947	-2.43204
C	1.91102	-2.42747	-3.85343
H	0.60585	-1.80775	-2.24940
C	4.23846	-1.76626	-3.65691
H	4.76496	-0.64035	-1.88153
C	3.21676	-2.41156	-4.36926
H	1.10258	-2.92559	-4.40032
H	5.25996	-1.74660	-4.05568
H	3.43636	-2.89485	-5.32829
C	0.50129	1.28319	-2.34278
O	0.59319	1.31124	-3.49272
C	-3.33020	4.44312	-0.67385
C	-3.21763	3.59049	0.43233
C	-2.32238	4.48385	-1.64322
H	-3.99700	3.58013	1.20118
H	-2.40260	5.17276	-2.49115
C	-2.11448	2.73379	0.52925
C	-1.22165	3.61565	-1.52935
H	-2.05654	2.07357	1.39705
H	-0.45214	3.66894	-2.30668
C	-1.12365	2.69623	-0.46918
I	1.14173	2.32754	1.93492
Cl	-4.75832	5.44771	-0.85282

E(DMF) = -3302.243433907241; G = 0.55541534

Pd(PPh₃)₂(CO)(PhICF₃) (**7g**)

Pd	0.31229	1.17053	-0.41206
P	-1.56194	-0.60537	0.12015
P	2.21084	-0.35490	-0.31188
C	-1.41948	-2.18246	-0.82775
C	-1.95191	-2.30480	-2.12852
C	-0.65059	-3.24462	-0.30516
C	-1.70762	-3.45631	-2.89143
H	-2.56430	-1.50093	-2.54801
C	-0.41022	-4.39251	-1.07080
H	-0.23975	-3.17724	0.70404
C	-0.93143	-4.50245	-2.36870
H	-2.12985	-3.53337	-3.90008
H	0.19694	-5.20094	-0.64741
H	-0.73507	-5.39806	-2.96984
C	-3.18441	0.08319	-0.42943
C	-3.23543	0.80078	-1.64394
C	-4.33269	0.03447	0.38253
C	-4.40462	1.46308	-2.03262
H	-2.33612	0.89131	-2.26035
C	-5.50268	0.70444	-0.00781
H	-4.30853	-0.50110	1.33647
C	-5.54090	1.42524	-1.20924
H	-4.41656	2.04539	-2.96014
H	-6.38518	0.67382	0.64277
H	-6.44296	1.97749	-1.49422
C	-1.90267	-1.17399	1.84001
C	-1.52759	-0.32968	2.90315
C	-2.54501	-2.39688	2.12409
C	-1.78145	-0.70493	4.23017
H	-1.00331	0.61141	2.69879
C	-2.79035	-2.77266	3.45178
H	-2.85505	-3.05529	1.30614
C	-2.40834	-1.92883	4.50808
H	-1.47670	-0.03864	5.04542
H	-3.28675	-3.72724	3.66319
H	-2.60300	-2.22589	5.54560
C	2.09839	-1.77267	0.85161
C	1.49106	-1.56745	2.10571
C	2.57912	-3.05174	0.50934
C	1.33660	-2.63811	2.99571
H	1.13835	-0.56735	2.37546
C	2.43529	-4.11686	1.41001
H	3.04542	-3.21845	-0.46641
C	1.80358	-3.91603	2.64784
H	0.83304	-2.47134	3.95410
H	2.80810	-5.11115	1.13743
H	1.67572	-4.75547	3.34186
C	3.76716	0.50540	0.13938
C	4.02444	1.76548	-0.43576
C	4.71122	-0.07471	1.00491
C	5.22263	2.43184	-0.15565
H	3.27252	2.23121	-1.08355
C	5.90648	0.60287	1.29112
H	4.51238	-1.05096	1.45848
C	6.16483	1.85285	0.71085
H	5.41330	3.41558	-0.59887
H	6.63691	0.15136	1.97316
H	7.09697	2.38260	0.94017
C	2.63771	-1.15816	-1.91725
C	1.60926	-1.77369	-2.65917
C	3.95572	-1.17844	-2.41530
C	1.89461	-2.40234	-3.87715
H	0.58183	-1.76209	-2.28746
C	4.23522	-1.80333	-3.64043
H	4.76324	-0.70379	-1.84905
C	3.20794	-2.41655	-4.37305
H	1.08235	-2.87553	-4.44013
H	5.26284	-1.80746	-4.02361
H	3.42963	-2.89840	-5.33233
C	0.51046	1.31297	-2.31926
O	0.59238	1.35546	-3.46954
C	-3.26685	4.53235	-0.58177
C	-3.18301	3.63016	0.49147

C	-2.23569	4.56200	-1.53239
H	-3.96481	3.61303	1.25779
H	-2.27132	5.28166	-2.35808
C	-2.11012	2.73721	0.57793
C	-1.16301	3.66178	-1.43986
H	-2.07870	2.04936	1.42512
H	-0.37775	3.71910	-2.20053
C	-1.10951	2.70266	-0.41082
I	1.16603	2.31618	1.95263
C	-4.48686	5.39676	-0.76328
F	-4.19543	6.58859	-1.33918
F	-5.40632	4.79468	-1.57587
F	-5.11964	5.65623	0.40557

E(DMF)= -3179.722679915784; G= 0.56808189

Pd(PPh₃)₂(CO)(PhICN) (**7h**)

Pd	0.28636	1.14644	-0.43032
P	-1.55939	-0.60417	0.09377
P	2.19486	-0.36344	-0.32206
C	-1.40637	-2.18939	-0.83821
C	-1.93780	-2.32790	-2.13771
C	-0.63498	-3.24268	-0.30214
C	-1.68925	-3.48736	-2.88687
H	-2.55237	-1.53089	-2.56691
C	-0.38990	-4.39823	-1.05460
H	-0.22669	-3.16255	0.70712
C	-0.90959	-4.52443	-2.35150
H	-2.11065	-3.57786	-3.89471
H	0.21912	-5.20010	-0.62163
H	-0.70979	-5.42621	-2.94213
C	-3.18362	0.06900	-0.46975
C	-3.23250	0.77449	-1.69103
C	-4.33830	0.01173	0.33237
C	-4.40877	1.41276	-2.09919
H	-2.32872	0.87063	-2.30006
C	-5.51430	0.66003	-0.07565
H	-4.31505	-0.51403	1.29169
C	-5.55250	1.36577	-1.28638
H	-4.42212	1.97590	-3.03877
H	-6.40247	0.62324	0.56661
H	-6.46448	1.89233	-1.58954
C	-1.90076	-1.15974	1.81770
C	-1.52366	-0.31358	2.87846
C	-2.54972	-2.37864	2.10465
C	-1.78292	-0.68266	4.20617
H	-0.99365	0.62406	2.67275
C	-2.80059	-2.74803	3.43302
H	-2.86040	-3.03895	1.28846
C	-2.41706	-1.90207	4.48704
H	-1.47679	-0.01481	5.01958
H	-3.30213	-3.69936	3.64679
H	-2.61627	-2.19402	5.52511
C	2.09687	-1.76822	0.85779
C	1.49644	-1.55180	2.11339
C	2.57961	-3.04913	0.52555
C	1.34918	-2.61412	3.01443
H	1.14428	-0.54942	2.37538
C	2.44326	-4.10565	1.43742
H	3.04077	-3.22465	-0.45111
C	1.81706	-3.89434	2.67627
H	0.85102	-2.43917	3.97420
H	2.81745	-5.10153	1.17277
H	1.69486	-4.72726	3.37909
C	3.74292	0.51806	0.11698
C	3.99939	1.76183	-0.49292
C	4.67975	-0.02935	1.01113
C	5.18907	2.44490	-0.21757
H	3.25327	2.20305	-1.16400
C	5.86668	0.66510	1.29191

H	4.48187	-0.99282	1.49168
C	6.12382	1.89908	0.67808
H	5.37855	3.41636	-0.68762
H	6.59122	0.23961	1.99657
H	7.04902	2.44255	0.90333
C	2.62803	-1.17907	-1.91918
C	1.60048	-1.77612	-2.67664
C	3.95476	-1.23176	-2.39184
C	1.89468	-2.41845	-3.88553
H	0.56698	-1.73997	-2.32401
C	4.24344	-1.87072	-3.60738
H	4.76158	-0.77152	-1.81289
C	3.21649	-2.46533	-4.35591
H	1.08314	-2.87721	-4.46130
H	5.27777	-1.90052	-3.97079
H	3.44558	-2.95823	-5.30783
C	0.53298	1.32781	-2.33340
O	0.61798	1.37579	-3.48338
C	-3.28269	4.53008	-0.55527
C	-3.19647	3.60855	0.51318
C	-2.25118	4.55593	-1.51755
H	-3.97645	3.59302	1.28219
H	-2.29138	5.28301	-2.33673
C	-2.13245	2.70804	0.57891
C	-1.19014	3.64402	-1.43871
H	-2.10088	2.00994	1.41753
H	-0.41128	3.69880	-2.20595
C	-1.13650	2.67519	-0.41715
I	1.16051	2.32959	1.92219
C	-4.40782	5.41088	-0.66555
N	-5.33978	6.11436	-0.76586

E(DMF)= -2934.867523354320; G= 0.56123235

Pd(PPh₃)₂(CO)(PhINO₂) (**7i**)

Pd	0.31343	1.16580	-0.40902
P	-1.55413	-0.59848	0.10328
P	2.21154	-0.35648	-0.31134
C	-1.41089	-2.17939	-0.83747
C	-1.94403	-2.30992	-2.13705
C	-0.64327	-3.23846	-0.30725
C	-1.70052	-3.46671	-2.89213
H	-2.55669	-1.50909	-2.56175
C	-0.40348	-4.39148	-1.06523
H	-0.23384	-3.16496	0.70213
C	-0.92450	-4.50945	-2.36248
H	-2.12345	-3.55073	-3.89989
H	0.20246	-5.19785	-0.63628
H	-0.72881	-5.40920	-2.95758
C	-3.17181	0.09546	-0.45431
C	-3.21806	0.80032	-1.67623
C	-4.31801	0.07054	0.36204
C	-4.38093	1.47303	-2.06815
H	-2.31988	0.87330	-2.29715
C	-5.47869	0.75595	-0.02832
H	-4.29714	-0.45472	1.32168
C	-5.51271	1.46453	-1.23737
H	-4.38981	2.03697	-3.00746
H	-6.35673	0.75041	0.62854
H	-6.40910	2.02708	-1.52076
C	-1.90146	-1.16308	1.82296
C	-1.51681	-0.32736	2.88928
C	-2.56186	-2.37758	2.10185
C	-1.78020	-0.70220	4.21460
H	-0.97896	0.60703	2.68969
C	-2.81659	-2.75311	3.42778
H	-2.87864	-3.02960	1.28136
C	-2.42576	-1.91748	4.48736
H	-1.46878	-0.04224	5.03242
H	-3.32714	-3.70107	3.63512

H	-2.62831	-2.21400	5.52347
C	2.10107	-1.77022	0.85639
C	1.49937	-1.56063	2.11243
C	2.57841	-3.05081	0.51505
C	1.34617	-2.62902	3.00533
H	1.15037	-0.55905	2.38124
C	2.43629	-4.11343	1.41887
H	3.04041	-3.22072	-0.46217
C	1.80940	-3.90856	2.65848
H	0.84688	-2.45919	3.96543
H	2.80642	-5.10898	1.14737
H	1.68268	-4.74610	3.35496
C	3.76652	0.50813	0.13570
C	4.02944	1.75932	-0.45603
C	4.70376	-0.06048	1.01617
C	5.22620	2.42851	-0.17702
H	3.28342	2.21675	-1.11638
C	5.89777	0.61997	1.30080
H	4.50089	-1.02988	1.48244
C	6.16157	1.86117	0.70449
H	5.42114	3.40547	-0.63316
H	6.62288	0.17754	1.99433
H	7.09267	2.39321	0.93258
C	2.63601	-1.16254	-1.91539
C	1.60457	-1.76165	-2.66621
C	3.95842	-1.20514	-2.40063
C	1.89097	-2.39627	-3.88094
H	0.57417	-1.73322	-2.30384
C	4.23909	-1.83627	-3.62222
H	4.76816	-0.74314	-1.82719
C	3.20859	-2.43310	-4.36396
H	1.07658	-2.85679	-4.45122
H	5.27006	-1.85815	-3.99558
H	3.43139	-2.91994	-5.32045
C	0.54771	1.33762	-2.31405
O	0.64702	1.39450	-3.46213
C	-3.29895	4.44119	-0.58873
C	-3.21204	3.56601	0.50204
C	-2.27389	4.51769	-1.53792
H	-4.01567	3.54520	1.24237
H	-2.35663	5.23294	-2.36112
C	-2.11135	2.71317	0.59939
C	-1.18167	3.64593	-1.43058
H	-2.05998	2.03367	1.45208
H	-0.39704	3.71201	-2.19090
C	-1.11102	2.69034	-0.39494
I	1.17692	2.32838	1.94669
N	-4.51072	5.26684	-0.76056
O	-5.44983	5.06807	0.00858
O	-4.52004	6.09017	-1.67303

E(DMF)= -3047.141209596414; G= 0.56409482

[Pd(PPh₃)₂(PhINH₂)][‡] (**10bTS**)

Pd	0.23422	0.90394	0.08985
P	-1.63520	-0.50261	0.21552
P	2.21896	-0.27446	-0.29801
C	-1.50079	-2.13088	-0.64964
C	-2.07726	-2.35845	-1.91611
C	-0.66458	-3.12436	-0.09387
C	-1.81068	-3.54546	-2.61567
H	-2.73451	-1.60426	-2.36118
C	-0.40710	-4.30941	-0.79280
H	-0.20792	-2.96749	0.88720
C	-0.97214	-4.52350	-2.06012
H	-2.26440	-3.70435	-3.60136
H	0.25121	-5.06304	-0.34583
H	-0.75922	-5.44676	-2.61194
C	-3.20266	0.18231	-0.47704
C	-3.11123	0.86923	-1.70601

C	-4.44987	0.09364	0.16819
C	-4.25229	1.41989	-2.30046
H	-2.12840	0.99902	-2.17545
C	-5.58863	0.67008	-0.41655
H	-4.53145	-0.41952	1.13147
C	-5.49514	1.32349	-1.65457
H	-4.16462	1.96541	-3.24548
H	-6.55548	0.60293	0.09772
H	-6.38727	1.77016	-2.10993
C	-2.09317	-1.01571	1.93094
C	-1.67650	-0.20296	3.00373
C	-2.83230	-2.18538	2.20202
C	-2.00000	-0.54719	4.32439
H	-1.07933	0.69355	2.79884
C	-3.14715	-2.53324	3.52334
H	-3.15370	-2.82895	1.37582
C	-2.73346	-1.71475	4.58714
H	-1.66874	0.09550	5.14857
H	-3.71666	-3.44877	3.72460
H	-2.98069	-1.98947	5.61961
C	2.26232	-1.72058	0.85309
C	1.73090	-1.53251	2.14695
C	2.72408	-2.99425	0.47587
C	1.64661	-2.60594	3.04202
H	1.34789	-0.54573	2.43009
C	2.63980	-4.06899	1.37537
H	3.12851	-3.15051	-0.52937
C	2.09509	-3.88061	2.65473
H	1.20910	-2.45094	4.03489
H	2.99349	-5.06112	1.06986
H	2.01665	-4.72582	3.34921
C	3.80252	0.59518	0.08006
C	3.94908	1.91392	-0.39555
C	4.84464	0.01381	0.82773
C	5.12609	2.63191	-0.14905
H	3.12208	2.37746	-0.94802
C	6.01826	0.73959	1.08561
H	4.73704	-1.00688	1.20946
C	6.16356	2.04607	0.59529
H	5.22735	3.65718	-0.52341
H	6.82374	0.28117	1.67262
H	7.07954	2.61277	0.80210
C	2.55005	-1.04903	-1.93777
C	1.44547	-1.56850	-2.64452
C	3.83916	-1.15351	-2.49742
C	1.62996	-2.20127	-3.88021
H	0.44183	-1.47865	-2.21766
C	4.01761	-1.77442	-3.74363
H	4.70261	-0.74977	-1.95750
C	2.91643	-2.30339	-4.43501
H	0.76184	-2.60963	-4.41025
H	5.02379	-1.84732	-4.17479
H	3.05993	-2.78795	-5.40793
C	-2.67424	4.21172	-1.31760
C	-1.32315	4.14785	-1.71554
C	-3.02997	3.66978	-0.05497
H	-1.01883	4.57434	-2.67955
H	-4.08039	3.68515	0.26092
C	-0.35326	3.56127	-0.88627
C	-2.07894	3.07448	0.76897
H	0.69865	3.56580	-1.19153
H	-2.38327	2.65295	1.73162
C	-0.73665	2.97361	0.33932
I	0.91570	2.92348	1.97463
N	-3.65029	4.73539	-2.16377
H	-3.32452	5.41009	-2.85101
H	-4.51143	5.03036	-1.71221

E(DMF)= -2784.658781556569; G= 0.57445130

[Pd(PPh₃)₂(PhIOH)][‡] (**10cTS**)

Pd	0.21932	0.92273	0.07225
P	-1.65099	-0.47892	0.22184
P	2.20521	-0.26262	-0.28643
C	-1.51887	-2.08986	-0.67751
C	-2.10021	-2.28737	-1.94684
C	-0.68172	-3.09743	-0.14932
C	-1.83815	-3.45766	-2.67563
H	-2.75903	-1.52323	-2.37165
C	-0.42840	-4.26594	-0.87758
H	-0.22091	-2.96598	0.83302
C	-0.99878	-4.44995	-2.14697
H	-2.29665	-3.59206	-3.66270
H	0.23111	-5.03051	-0.45135
H	-0.78957	-5.36027	-2.72129
C	-3.24427	0.20006	-0.41277
C	-3.20343	0.89115	-1.64207
C	-4.46455	0.10903	0.28209
C	-4.36844	1.44245	-2.18772
H	-2.23990	1.02357	-2.14964
C	-5.62627	0.68657	-0.25411
H	-4.50693	-0.40742	1.24627
C	-5.58418	1.34400	-1.49262
H	-4.32138	1.98847	-3.13589
H	-6.57088	0.61886	0.29957
H	-6.49293	1.79528	-1.90767
C	-2.05414	-1.02088	1.94198
C	-1.63438	-0.20518	3.01131
C	-2.74608	-2.21690	2.22094
C	-1.90167	-0.57666	4.33698
H	-1.07716	0.71496	2.79893
C	-3.00444	-2.59207	3.54704
H	-3.07441	-2.85984	1.39717
C	-2.58282	-1.77384	4.60781
H	-1.56726	0.06754	5.15864
H	-3.53603	-3.52873	3.75410
H	-2.78447	-2.07088	5.64407
C	2.22109	-1.72052	0.85049
C	1.66953	-1.54272	2.13708
C	2.68411	-2.99234	0.46858
C	1.56269	-2.62462	3.01951
H	1.28839	-0.55661	2.42402
C	2.57862	-4.07551	1.35558
H	3.10547	-3.14016	-0.53092
C	2.01114	-3.89760	2.62667
H	1.10674	-2.47715	4.00507
H	2.93308	-5.06625	1.04655
H	1.91514	-4.74978	3.31031
C	3.78791	0.59076	0.13053
C	3.96330	1.90645	-0.34410
C	4.80205	-0.00007	0.90872
C	5.14043	2.61206	-0.06511
H	3.15880	2.37797	-0.92241
C	5.97555	0.71342	1.19903
H	4.67282	-1.01869	1.28913
C	6.14924	2.01705	0.71069
H	5.26413	3.63513	-0.43872
H	6.75869	0.24726	1.80970
H	7.06495	2.57419	0.94278
C	2.55915	-1.02196	-1.92803
C	1.46412	-1.53248	-2.65610
C	3.85626	-1.12132	-2.46953
C	1.66626	-2.15076	-3.89638
H	0.45444	-1.44703	-2.24221
C	4.05222	-1.72758	-3.72027
H	4.71188	-0.72503	-1.91187
C	2.96060	-2.24696	-4.43372
H	0.80599	-2.55247	-4.44397
H	5.06446	-1.79669	-4.13765
H	3.11787	-2.71992	-5.41019
C	-2.59673	4.22822	-1.41314
C	-1.25481	4.13307	-1.81296
C	-2.98649	3.74083	-0.14510

H	-0.94148	4.52836	-2.78850
H	-4.04133	3.79863	0.14192
C	-0.29614	3.56104	-0.95574
C	-2.04892	3.15704	0.70169
H	0.75808	3.53991	-1.25053
H	-2.36287	2.76674	1.67441
C	-0.70307	3.02586	0.28616
I	0.91210	2.96566	1.92897
O	-3.56889	4.77227	-2.20519
H	-3.15597	5.09209	-3.02198

E(DMF)= -2804.538088480578; G= 0.56310563

[Pd(PPh₃)₂(PhICH₃)][†] (10dTS)

Pd	0.22066	0.89167	0.08073
P	-1.65631	-0.48273	0.22601
P	2.21415	-0.26123	-0.30791
C	-1.51669	-2.11302	-0.63895
C	-2.10268	-2.35793	-1.89730
C	-0.66901	-3.09548	-0.08110
C	-1.83132	-3.54873	-2.58895
H	-2.77270	-1.61625	-2.34380
C	-0.40700	-4.28457	-0.77128
H	-0.20707	-2.92681	0.89536
C	-0.97934	-4.51422	-2.03250
H	-2.29245	-3.72018	-3.56907
H	0.26048	-5.02867	-0.32222
H	-0.76267	-5.44021	-2.57820
C	-3.21796	0.20742	-0.47026
C	-3.13460	0.82155	-1.73782
C	-4.45145	0.19639	0.20652
C	-4.27491	1.36413	-2.34075
H	-2.16005	0.89341	-2.23603
C	-5.58625	0.77357	-0.38510
H	-4.52460	-0.25958	1.19884
C	-5.50520	1.34466	-1.66399
H	-4.19781	1.82865	-3.33006
H	-6.54145	0.76850	0.15451
H	-6.39617	1.78470	-2.12775
C	-2.11817	-1.00287	1.93812
C	-1.68503	-0.20933	3.01836
C	-2.86944	-2.16729	2.19818
C	-2.00148	-0.56910	4.33682
H	-1.08073	0.68393	2.82035
C	-3.17743	-2.53073	3.51674
H	-3.20428	-2.79504	1.36515
C	-2.74486	-1.73273	4.58865
H	-1.65687	0.05755	5.16779
H	-3.75515	-3.44287	3.70975
H	-2.98528	-2.02052	5.61916
C	2.26117	-1.71348	0.83746
C	1.73192	-1.53533	2.13345
C	2.73370	-2.98172	0.45507
C	1.66080	-2.61239	3.02550
H	1.34001	-0.55353	2.42137
C	2.66227	-4.06036	1.35106
H	3.13813	-3.13105	-0.55112
C	2.12017	-3.88153	2.63284
H	1.22547	-2.46490	4.02047
H	3.02457	-5.04796	1.04096
H	2.05256	-4.72972	3.32483
C	3.80118	0.60059	0.07741
C	3.96805	1.90964	-0.41838
C	4.82464	0.02511	0.85509
C	5.14494	2.62354	-0.16019
H	3.15807	2.36902	-0.99884
C	5.99814	0.74697	1.12440
H	4.70326	-0.98837	1.25130
C	6.16280	2.04385	0.61565
H	5.26195	3.64104	-0.55075

H	6.78846	0.29233	1.73455
H	7.07856	2.60755	0.83118
C	2.54580	-1.03285	-1.94862
C	1.44019	-1.54841	-2.65659
C	3.83583	-1.14426	-2.50454
C	1.62466	-2.18343	-3.89116
H	0.43639	-1.45446	-2.23024
C	4.01418	-1.76705	-3.74980
H	4.69979	-0.74482	-1.96213
C	2.91195	-2.29143	-4.44304
H	0.75630	-2.58920	-4.42282
H	5.02094	-1.84544	-4.17858
H	3.05544	-2.77744	-5.41521
C	-2.59079	4.18388	-1.35368
C	-1.24372	4.08237	-1.73875
C	-2.95650	3.68922	-0.07900
H	-0.92820	4.46524	-2.71769
H	-4.00808	3.72569	0.23134
C	-0.27180	3.53215	-0.88188
C	-2.01905	3.12441	0.78367
H	0.78283	3.51856	-1.17577
H	-2.32784	2.73671	1.75914
C	-0.67212	3.01374	0.37010
I	0.92638	2.91264	1.98229
C	-3.61796	4.83332	-2.24854
H	-3.33945	4.75160	-3.31444
H	-4.61184	4.37253	-2.11542
H	-3.72397	5.91234	-2.01848

E(DMF)= -2768.605822001488; G= 0.58416282

[Pd(PPh₃)₂(PhIF)][‡] (10eTS)

Pd	0.23637	0.86177	0.16856
P	-1.66242	-0.49459	0.24532
P	2.23333	-0.25549	-0.30495
C	-1.51364	-2.15908	-0.54653
C	-2.10961	-2.48062	-1.78228
C	-0.65284	-3.09896	0.06172
C	-1.83040	-3.70660	-2.40690
H	-2.79061	-1.77097	-2.26372
C	-0.38338	-4.32260	-0.56102
H	-0.18295	-2.86518	1.02157
C	-0.96284	-4.62852	-1.80320
H	-2.29641	-3.93962	-3.37190
H	0.29556	-5.03269	-0.07592
H	-0.73952	-5.58156	-2.29686
C	-3.13716	0.22892	-0.58930
C	-2.93334	0.77742	-1.87427
C	-4.40901	0.32902	0.00299
C	-3.98945	1.37996	-2.56663
H	-1.92885	0.75223	-2.31503
C	-5.46021	0.95763	-0.68415
H	-4.57921	-0.07253	1.00712
C	-5.25709	1.47638	-1.97069
H	-3.81519	1.80828	-3.55968
H	-6.44470	1.04221	-0.20728
H	-6.07803	1.97137	-2.50212
C	-2.26121	-0.94941	1.93227
C	-1.80825	-0.19886	3.03437
C	-3.13766	-2.03278	2.14809
C	-2.23513	-0.51656	4.33265
H	-1.10344	0.62501	2.86766
C	-3.55897	-2.35224	3.44633
H	-3.48044	-2.63137	1.29653
C	-3.11044	-1.59362	4.54035
H	-1.87475	0.07435	5.18287
H	-4.23673	-3.19966	3.60723
H	-3.43937	-1.84724	5.55509
C	2.36503	-1.71868	0.81585
C	1.90555	-1.56351	2.14126

C	2.84320	-2.97226	0.39427
C	1.91625	-2.64852	3.02658
H	1.50537	-0.59357	2.45930
C	2.85225	-4.05892	1.28351
H	3.19236	-3.10285	-0.63515
C	2.38557	-3.90221	2.59732
H	1.54109	-2.52019	4.04866
H	3.21960	-5.03476	0.94356
H	2.38383	-4.75587	3.28575
C	3.81964	0.63534	0.00961
C	3.92722	1.95952	-0.46151
C	4.90112	0.06516	0.70864
C	5.10167	2.69484	-0.25720
H	3.07360	2.41293	-0.98041
C	6.07276	0.80780	0.92437
H	4.82666	-0.96006	1.08565
C	6.17755	2.12032	0.44004
H	5.17186	3.72376	-0.62850
H	6.90863	0.35738	1.47379
H	7.09225	2.69987	0.61420
C	2.48979	-0.99082	-1.97531
C	1.36351	-1.54565	-2.61836
C	3.74121	-1.02634	-2.62179
C	1.49084	-2.14365	-3.87805
H	0.38829	-1.51086	-2.12321
C	3.86112	-1.61211	-3.89201
H	4.62129	-0.59585	-2.13154
C	2.73971	-2.17517	-4.52078
H	0.60697	-2.57953	-4.35807
H	4.83786	-1.62988	-4.39125
H	2.83739	-2.63192	-5.51250
C	-2.63188	4.05717	-1.23063
C	-1.30515	4.01671	-1.66034
C	-3.01292	3.58841	0.03694
H	-1.04136	4.40832	-2.64817
H	-4.06785	3.61568	0.32655
C	-0.32134	3.49254	-0.80123
C	-2.04535	3.05248	0.88623
H	0.73056	3.50200	-1.10337
H	-2.33427	2.66556	1.86784
C	-0.70105	2.96440	0.45477
I	0.92526	2.88963	2.05044
F	-3.57811	4.56106	-2.05265

E(DMF)= -2828.563225761498; G= 0.54876870

[Pd(PPh₃)₂(PhICl)][‡] (10fTS)

Pd	0.21911	0.86261	0.13646
P	-1.67418	-0.49245	0.23865
P	2.22170	-0.24961	-0.32508
C	-1.51514	-2.14864	-0.56952
C	-2.11826	-2.46704	-1.80242
C	-0.64065	-3.08468	0.02490
C	-1.83257	-3.68604	-2.43786
H	-2.81073	-1.76111	-2.27272
C	-0.36448	-4.30119	-0.60860
H	-0.16640	-2.85375	0.98320
C	-0.95126	-4.60383	-1.84811
H	-2.30477	-3.91688	-3.40039
H	0.32491	-5.00832	-0.13397
H	-0.72321	-5.55119	-2.35047
C	-3.16432	0.22460	-0.57173
C	-2.98313	0.77232	-1.86063
C	-4.42606	0.32096	0.04201
C	-4.05330	1.36637	-2.53766
H	-1.98557	0.75144	-2.31706
C	-5.49062	0.94540	-0.62866
H	-4.57827	-0.08083	1.04890
C	-5.31092	1.46033	-1.91994
H	-3.89830	1.79261	-3.53459

H	-6.46713	1.02836	-0.13533
H	-6.14124	1.95352	-2.43819
C	-2.25436	-0.97040	1.92578
C	-1.81133	-0.22038	3.03199
C	-3.11214	-2.06975	2.13618
C	-2.22798	-0.55549	4.32930
H	-1.12297	0.61797	2.87025
C	-3.52295	-2.40673	3.43323
H	-3.44925	-2.66629	1.28101
C	-3.08333	-1.64938	4.53176
H	-1.87553	0.03562	5.18271
H	-4.18585	-3.26662	3.58962
H	-3.40426	-1.91656	5.54557
C	2.35534	-1.69635	0.81839
C	1.87856	-1.52983	2.13624
C	2.84540	-2.95207	0.41686
C	1.88263	-2.60536	3.03312
H	1.46903	-0.55919	2.43936
C	2.84795	-4.02921	1.31759
H	3.20777	-3.09301	-0.60649
C	2.36304	-3.86125	2.62335
H	1.49269	-2.46790	4.04840
H	3.22415	-5.00678	0.99268
H	2.35534	-4.70787	3.32039
C	3.80083	0.65617	-0.01886
C	3.91612	1.95768	-0.54838
C	4.86554	0.12407	0.73340
C	5.08111	2.70804	-0.34657
H	3.07574	2.38098	-1.11288
C	6.02773	0.88272	0.94660
H	4.78548	-0.88355	1.15421
C	6.13995	2.17228	0.40614
H	5.15740	3.71889	-0.76348
H	6.85041	0.46234	1.53812
H	7.04687	2.76446	0.57821
C	2.48957	-1.01167	-1.98146
C	1.36159	-1.54257	-2.64075
C	3.75492	-1.10128	-2.59497
C	1.50020	-2.17155	-3.88438
H	0.37652	-1.46543	-2.17020
C	3.88687	-1.71835	-3.84886
H	4.63598	-0.68908	-2.09091
C	2.76293	-2.25822	-4.49364
H	0.61489	-2.58897	-4.37768
H	4.87439	-1.77934	-4.32267
H	2.87003	-2.73950	-5.47274
C	-2.54493	4.12432	-1.26926
C	-1.19957	4.06826	-1.64885
C	-2.96892	3.62273	-0.02236
H	-0.88345	4.47724	-2.61355
H	-4.02958	3.65094	0.24398
C	-0.25212	3.51559	-0.76793
C	-2.03775	3.06167	0.84986
H	0.81004	3.52489	-1.03189
H	-2.36640	2.65967	1.81276
C	-0.67843	2.96961	0.46670
I	0.88697	2.86026	2.09697
Cl	-3.72135	4.84066	-2.35192

E(DMF)= -3188.911430216371; G= 0.54665534

[Pd(PPh₃)₂(PhICF₃)₃][‡] (**10gTS**)

Pd	0.31586	0.91403	0.26204
P	-1.49892	-0.53060	0.44354
P	2.39437	-0.12542	-0.02663
C	-1.23355	-2.18472	-0.34172
C	-1.78320	-2.53855	-1.59027
C	-0.32851	-3.07236	0.28042
C	-1.41757	-3.74337	-2.21119
H	-2.50042	-1.87422	-2.08354

C	0.02827	-4.27517	-0.33927
H	0.10256	-2.81467	1.25158
C	-0.50733	-4.61285	-1.59251
H	-1.85189	-4.00225	-3.18415
H	0.73923	-4.94368	0.15895
H	-0.21811	-5.54989	-2.08213
C	-3.06786	0.05470	-0.32120
C	-2.98646	0.58702	-1.62582
C	-4.30515	0.06921	0.34889
C	-4.12936	1.07813	-2.26641
H	-2.01112	0.64037	-2.12515
C	-5.44392	0.59310	-0.28426
H	-4.37829	-0.32173	1.36862
C	-5.36236	1.08654	-1.59438
H	-4.05047	1.49265	-3.27577
H	-6.40138	0.61137	0.25116
H	-6.25102	1.49991	-2.08477
C	-1.98590	-1.00742	2.16042
C	-1.61754	-0.16290	3.22524
C	-2.70374	-2.18933	2.43592
C	-1.96417	-0.49000	4.54479
H	-1.04361	0.74718	3.01537
C	-3.04383	-2.51866	3.75535
H	-2.98961	-2.85507	1.61392
C	-2.67512	-1.67013	4.81244
H	-1.67050	0.17634	5.36453
H	-3.59744	-3.44283	3.96087
H	-2.94129	-1.93088	5.84375
C	2.51527	-1.50751	1.19524
C	1.94796	-1.30012	2.47075
C	3.07576	-2.75960	0.88556
C	1.92723	-2.33391	3.41472
H	1.48715	-0.33287	2.70089
C	3.05346	-3.79515	1.83336
H	3.50937	-2.93235	-0.10478
C	2.47419	-3.58849	3.09452
H	1.46240	-2.16633	4.39309
H	3.48316	-4.77178	1.58010
H	2.44517	-4.40449	3.82681
C	3.89955	0.87583	0.34273
C	4.01040	2.13643	-0.27961
C	4.90590	0.46070	1.23559
C	5.11359	2.96100	-0.02773
H	3.21518	2.46863	-0.95879
C	6.00499	1.29480	1.49835
H	4.82934	-0.51423	1.72813
C	6.11340	2.54281	0.86732
H	5.18635	3.93876	-0.51795
H	6.78125	0.96543	2.20019
H	6.97044	3.19399	1.07737
C	2.80803	-0.94474	-1.62331
C	1.75182	-1.55674	-2.33019
C	4.11385	-0.99133	-2.15032
C	2.00182	-2.22003	-3.53819
H	0.73520	-1.51284	-1.92627
C	4.35665	-1.64357	-3.36921
H	4.93904	-0.51750	-1.60744
C	3.30413	-2.26122	-4.06299
H	1.17233	-2.69818	-4.07180
H	5.37434	-1.66992	-3.77804
H	3.49789	-2.76716	-5.01611
C	-2.43121	3.98316	-1.43071
C	-1.05767	3.94214	-1.71792
C	-2.89797	3.54844	-0.17124
H	-0.68870	4.29372	-2.68758
H	-3.97018	3.55439	0.04487
C	-0.14159	3.48966	-0.75627
C	-2.00577	3.08074	0.79057
H	0.93383	3.52814	-0.95460
H	-2.37473	2.73363	1.76021
C	-0.62380	3.01213	0.49069
I	0.83756	3.03905	2.18473
C	-3.37371	4.54436	-2.46280

F	-3.18729	5.87796	-2.64521
F	-3.18532	3.96766	-3.68489
F	-4.67546	4.36781	-2.13822

E(DMF)= -3066.391134408485; G= 0.55899176

[Pd(PPh₃)₂(PhICN)][‡] (10hTS)

Pd	0.19939	0.85120	0.14195
P	-1.70966	-0.48215	0.23920
P	2.21031	-0.25708	-0.32165
C	-1.53088	-2.12879	-0.58319
C	-2.14552	-2.45429	-1.80803
C	-0.63367	-3.05087	-0.00133
C	-1.84747	-3.66736	-2.44947
H	-2.85664	-1.75985	-2.26734
C	-0.34539	-4.26140	-0.64060
H	-0.15174	-2.81352	0.95161
C	-0.94315	-4.57098	-1.87312
H	-2.32854	-3.90457	-3.40599
H	0.36139	-4.95809	-0.17621
H	-0.70597	-5.51339	-2.38044
C	-3.20011	0.23930	-0.56360
C	-3.03247	0.76803	-1.86222
C	-4.44822	0.36904	0.07238
C	-4.10169	1.38056	-2.52470
H	-2.04482	0.72173	-2.33782
C	-5.51195	1.00886	-0.58547
H	-4.58974	-0.01777	1.08664
C	-5.34510	1.50941	-1.88429
H	-3.95914	1.79629	-3.52761
H	-6.47662	1.11831	-0.07451
H	-6.17016	2.02165	-2.39177
C	-2.28251	-0.98249	1.92128
C	-1.81867	-0.26518	3.04021
C	-3.15145	-2.07642	2.11346
C	-2.22518	-0.62763	4.33348
H	-1.12326	0.56963	2.89127
C	-3.55299	-2.43994	3.40600
H	-3.50378	-2.64800	1.24747
C	-3.09168	-1.71574	4.51793
H	-1.85670	-0.06247	5.19756
H	-4.22478	-3.29526	3.54848
H	-3.40475	-2.00430	5.52827
C	2.36556	-1.69599	0.82745
C	1.89189	-1.52974	2.14647
C	2.86618	-2.94821	0.42805
C	1.91007	-2.60204	3.04703
H	1.47378	-0.56228	2.44812
C	2.88245	-4.02217	1.33239
H	3.22540	-3.08953	-0.59629
C	2.40126	-3.85444	2.63956
H	1.52295	-2.46511	4.06344
H	3.26676	-4.99710	1.00925
H	2.40467	-4.69871	3.33940
C	3.77620	0.67415	-0.02684
C	3.88556	1.95943	-0.59647
C	4.83465	0.17891	0.75854
C	5.03678	2.73121	-0.39768
H	3.05238	2.35289	-1.19236
C	5.98331	0.95941	0.96788
H	4.75994	-0.81596	1.20950
C	6.08856	2.23331	0.39049
H	5.10799	3.72907	-0.84557
H	6.80088	0.56803	1.58572
H	6.98462	2.84245	0.55975
C	2.47515	-1.01680	-1.97835
C	1.34105	-1.50461	-2.65936
C	3.74814	-1.15012	-2.56787
C	1.48039	-2.13491	-3.90256
H	0.35117	-1.39387	-2.20579

C	3.88142	-1.76920	-3.82026
H	4.63315	-0.76882	-2.04660
C	2.75050	-2.26613	-4.48745
H	0.59051	-2.51855	-4.41445
H	4.87457	-1.86507	-4.27590
H	2.85862	-2.74862	-5.46579
C	-2.48204	4.06508	-1.30667
C	-1.11000	4.01236	-1.63536
C	-2.91585	3.58736	-0.03885
H	-0.76921	4.39826	-2.60192
H	-3.98195	3.60605	0.20697
C	-0.17869	3.49648	-0.72455
C	-2.00448	3.06237	0.86725
H	0.89028	3.51731	-0.95627
H	-2.34720	2.68215	1.83397
C	-0.63479	2.96343	0.51182
I	0.87710	2.85590	2.15191
C	-3.43204	4.57720	-2.24465
N	-4.21787	4.97347	-3.01984

E(DMF)= -2821.537613451037; G= 0.55576757

[Pd(PPh₃)₂(PhINO₂)][‡] (10iTS)

Pd	0.26125	0.69353	1.00457
P	-1.67199	-0.57563	0.68230
P	2.16454	-0.34512	0.09385
C	-1.36625	-2.33575	0.21269
C	-1.87669	-2.93052	-0.95640
C	-0.51427	-3.08483	1.05016
C	-1.52003	-4.24640	-1.29070
H	-2.53381	-2.35626	-1.61755
C	-0.15720	-4.39570	0.71442
H	-0.10957	-2.62420	1.95747
C	-0.65248	-4.97761	-0.46512
H	-1.91519	-4.69741	-2.20886
H	0.52630	-4.95399	1.36431
H	-0.36199	-5.99851	-0.73852
C	-2.62320	0.07673	-0.75217
C	-1.88997	0.34582	-1.92808
C	-3.99468	0.38898	-0.71022
C	-2.52230	0.89926	-3.04659
H	-0.81655	0.13684	-1.95858
C	-4.62182	0.95866	-1.83010
H	-4.57211	0.20598	0.20212
C	-3.89035	1.21340	-2.99863
H	-1.93445	1.12144	-3.94362
H	-5.68488	1.22200	-1.78126
H	-4.37450	1.68835	-3.85904
C	-2.91911	-0.77109	2.02970
C	-2.80214	0.02848	3.18211
C	-3.96730	-1.70995	1.94293
C	-3.73495	-0.08794	4.22400
H	-1.96048	0.72698	3.26588
C	-4.89734	-1.82646	2.98517
H	-4.04820	-2.35323	1.05884
C	-4.78560	-1.01229	4.12488
H	-3.63366	0.53827	5.11864
H	-5.71087	-2.55879	2.91102
H	-5.51311	-1.10759	4.94049
C	2.73374	-1.95894	0.78489
C	2.55987	-2.15408	2.16940
C	3.33666	-2.97422	0.01759
C	2.97067	-3.34912	2.77637
H	2.08029	-1.36399	2.76235
C	3.73610	-4.17392	0.62319
H	3.48224	-2.83720	-1.05926
C	3.55241	-4.36541	2.00186
H	2.82483	-3.49221	3.85388
H	4.19231	-4.96472	0.01527
H	3.86302	-5.30638	2.47145

C	3.75368	0.59914	-0.02587
C	3.90512	1.76818	0.74214
C	4.81103	0.17569	-0.85688
C	5.09602	2.51028	0.67839
H	3.08453	2.08984	1.39490
C	5.99804	0.91710	-0.92040
H	4.70256	-0.73131	-1.46130
C	6.14215	2.08676	-0.15392
H	5.20065	3.42225	1.27766
H	6.81592	0.58331	-1.57050
H	7.07144	2.66653	-0.20851
C	1.75628	-0.67822	-1.67001
C	1.12650	-1.87493	-2.06840
C	1.87611	0.37642	-2.60153
C	0.63468	-2.01352	-3.37432
H	0.99564	-2.69347	-1.35587
C	1.37831	0.23471	-3.90318
H	2.34696	1.31789	-2.29783
C	0.75533	-0.96212	-4.29495
H	0.13851	-2.94724	-3.66250
H	1.47010	1.06597	-4.61234
H	0.35706	-1.06876	-5.31046
C	-1.83543	3.66795	-1.23721
C	-0.44001	3.54690	-1.23402
C	-2.60061	3.38599	-0.08552
H	0.12039	3.80247	-2.13701
H	-3.68572	3.50084	-0.12977
C	0.21586	3.13334	-0.06724
C	-1.96842	2.93207	1.06499
H	1.30879	3.13757	-0.02231
H	-2.55646	2.67821	1.95169
C	-0.56044	2.72940	1.06184
I	0.50163	2.70777	3.04210
N	-2.51220	4.10955	-2.45828
O	-3.71225	4.37929	-2.38655
O	-1.84591	4.17536	-3.49420

E(DMF)= -2933.812558623218; G= 0.55698152

Pd(PPh₃)₂(PhINH₂) (10b)

Pd	-0.85861	-0.73498	0.13656
P	-0.57144	1.46836	0.84530
P	1.37284	-1.19052	-0.64535
H	-1.30527	4.67182	-3.88203
H	2.40643	2.18450	-5.18966
H	0.33532	0.78168	-5.03949
H	2.95842	-4.67905	-3.90785
H	-2.09230	2.29391	-3.82169
C	2.24383	1.53269	-4.32298
C	1.08368	0.74682	-4.23865
C	-1.16322	4.06694	-2.97827
C	-1.60647	2.73703	-2.94464
C	2.54343	-4.48003	-2.91266
H	2.46581	-2.33552	-3.22314
H	2.50829	-6.57079	-2.33398
H	4.10563	2.08712	-3.35201
C	3.19434	1.47962	-3.29291
C	0.86480	-0.07254	-3.12467
H	-0.04960	-0.67385	-3.05056
C	2.26682	-3.15793	-2.52840
H	-0.17979	5.66037	-1.87503
C	2.29101	-5.53969	-2.03085
C	-0.53187	4.62244	-1.85304
C	-1.41799	1.96011	-1.79295
H	-1.73949	0.91222	-1.77089
C	2.98757	0.64742	-2.18170
C	1.81638	-0.12700	-2.08286
I	-1.88676	-2.69412	-1.37090
C	1.72961	-2.89451	-1.25725
C	1.75435	-5.27755	-0.75901

C	-0.34579	3.85034	-0.69817
H	3.73600	0.61562	-1.38448
C	-0.78947	2.51167	-0.66036
H	1.98210	2.07895	-0.42363
H	1.54350	-6.10265	-0.06871
C	1.46965	-3.96286	-0.37557
H	0.15434	4.28362	0.17451
H	4.33732	-1.59977	-0.73875
H	-3.61333	0.93381	-0.35428
H	4.22587	2.69534	0.44091
C	2.12239	2.24029	0.64798
H	1.03020	-3.76101	0.60817
H	-2.39677	3.86671	0.91906
C	4.06840	-1.30200	0.28089
C	3.38473	2.59464	1.13679
C	2.72141	-1.03760	0.60334
C	-3.75324	0.29168	0.52241
H	-5.69780	1.15233	0.93850
C	1.02922	2.09219	1.52475
C	-4.93966	0.42425	1.25648
H	6.10577	-1.41624	1.00721
C	-2.75160	-0.60842	0.91841
C	5.05982	-1.21307	1.26693
C	-2.53783	3.29239	1.83959
C	-1.79696	2.11728	2.05938
C	2.37818	-0.74145	1.93479
H	1.32636	-0.57072	2.18751
C	3.57323	2.81044	2.51024
H	-4.05969	4.63016	2.60448
H	4.56315	3.07985	2.89600
C	-3.48205	3.71621	2.78692
C	-5.16545	-0.34927	2.41597
C	-2.99884	-1.42269	2.03791
C	4.71263	-0.88494	2.58795
C	1.21858	2.32862	2.89983
C	3.36930	-0.66192	2.92227
H	-2.25676	-2.16696	2.35532
C	2.48503	2.68490	3.38656
C	-4.18116	-1.29452	2.78193
C	-2.01365	1.37283	3.23595
H	5.48951	-0.81662	3.35884
H	0.37710	2.23845	3.59375
H	-1.46973	0.43609	3.39241
H	3.08935	-0.41650	3.95250
C	-3.69597	2.97056	3.95538
H	-4.34380	-1.93309	3.66057
C	-2.95752	1.79749	4.17779
H	2.61948	2.86748	4.45952
H	-4.44304	3.29666	4.68932
H	-3.12975	1.19629	5.07802
N	-6.35356	-0.22244	3.14383
H	-6.79990	0.68848	3.06814
H	-6.29109	-0.52312	4.11310

E(DMF)= -2784.691143910871; G= 0.57576604

Pd(PPh₃)₂(PhIOH) (10c)

Pd	-0.85665	-0.71189	0.15087
P	-0.55551	1.49486	0.84494
P	1.36933	-1.17439	-0.64101
H	-1.29805	4.66739	-3.90123
H	2.42704	2.19615	-5.18257
H	0.33669	0.82335	-5.02434
H	2.88407	-4.67505	-3.92418
H	-2.11866	2.30181	-3.81071
C	2.25936	1.54532	-4.31615
C	1.08847	0.77613	-4.22741
C	-1.15253	4.06777	-2.99454
C	-1.61451	2.74476	-2.94391
C	2.48776	-4.47242	-2.92213

H	2.41545	-2.32806	-3.23474
H	2.45210	-6.56212	-2.33987
H	4.13333	2.07209	-3.35321
C	3.21402	1.47725	-3.29069
C	0.86365	-0.04219	-3.11377
H	-0.05840	-0.63115	-3.03646
C	2.22499	-3.14829	-2.53516
H	-0.13214	5.65581	-1.91762
C	2.24565	-5.52948	-2.03441
C	-0.49817	4.62313	-1.88253
C	-1.42129	1.97455	-1.78856
H	-1.75635	0.93122	-1.75412
C	3.00094	0.64627	-2.17984
C	1.81966	-0.11215	-2.07698
I	-1.89616	-2.66636	-1.35560
C	1.71225	-2.88039	-1.25496
C	1.73347	-5.26275	-0.75346
C	-0.30789	3.85808	-0.72359
H	3.75228	0.60323	-1.38591
C	-0.76955	2.52623	-0.66909
H	2.00414	2.08515	-0.42498
H	1.53096	-6.08571	-0.05814
C	1.46304	-3.94604	-0.36688
H	0.20781	4.29209	0.13956
H	4.32899	-1.60832	-0.73151
H	-3.62321	0.94145	-0.31738
H	4.25091	2.68720	0.44137
C	2.14396	2.24753	0.64647
H	1.04322	-3.74059	0.62466
H	-2.36576	3.90329	0.89271
C	4.06182	-1.30798	0.28782
C	3.40819	2.59375	1.13634
C	2.71683	-1.03260	0.60969
C	-3.75327	0.29441	0.55703
H	-5.71725	1.12044	0.98234
C	1.04888	2.10883	1.52229
C	-4.94484	0.40220	1.29233
H	6.09772	-1.43874	1.01521
C	-2.74118	-0.59292	0.95134
C	5.05339	-1.22695	1.27438
C	-2.51803	3.33320	1.81418
C	-1.78121	2.15866	2.04922
C	2.37528	-0.73367	1.94096
H	1.32483	-0.55463	2.19368
C	3.59644	2.81016	2.50968
H	-4.04683	4.67660	2.55527
H	4.58781	3.07292	2.89629
C	-3.47251	3.76279	2.74883
C	-5.14477	-0.38689	2.43843
C	-2.97225	-1.41454	2.07128
C	4.70820	-0.89582	2.59516
C	1.23789	2.34633	2.89728
C	3.36657	-0.66202	2.92888
H	-2.21677	-2.14750	2.38266
C	2.50631	2.69400	3.38495
C	-4.15609	-1.31342	2.81657
C	-2.01124	1.42145	3.22808
H	5.48522	-0.83376	3.36641
H	0.39484	2.26378	3.59024
H	-1.47050	0.48475	3.39619
H	3.08802	-0.41467	3.95902
C	-3.70167	3.02260	3.91764
H	-4.32873	-1.94555	3.69516
C	-2.96665	1.85054	4.15596
H	2.64077	2.87732	4.45774
H	-4.46000	3.34966	4.63915
H	-3.15455	1.25253	5.05476
O	-6.27139	-0.29460	3.21201
H	-6.85978	0.36301	2.81085

E(DMF)= -2804.571460621916; G= 0.56408040

Pd(PPh₃)₂(PhICH₃) (10d)

Pd	-0.85681	-0.71860	0.13992
P	-0.56354	1.48734	0.83798
P	1.37315	-1.17957	-0.64609
H	-1.28416	4.67469	-3.90093
H	2.43481	2.19287	-5.18524
H	0.35162	0.80812	-5.03676
H	2.91165	-4.67855	-3.91963
H	-2.09116	2.30393	-3.82800
C	2.26655	1.54150	-4.31934
C	1.09964	0.76567	-4.23602
C	-1.14278	4.07194	-2.99567
C	-1.59714	2.74597	-2.95498
C	2.50711	-4.47651	-2.92076
H	2.43904	-2.33181	-3.23198
H	2.46512	-6.56670	-2.34063
H	4.13281	2.07912	-3.34748
C	3.21649	1.47923	-3.28920
C	0.87375	-0.05320	-3.12304
H	-0.04559	-0.64692	-3.04998
C	2.24192	-3.15257	-2.53483
H	-0.14201	5.66160	-1.90269
C	2.25678	-5.53419	-2.03602
C	-0.50188	4.62651	-1.87539
C	-1.40980	1.97186	-1.80123
H	-1.74021	0.92693	-1.77385
C	3.00260	0.64756	-2.17898
C	1.82496	-0.11723	-2.08144
I	-1.89423	-2.67183	-1.37164
C	1.71834	-2.88547	-1.25881
C	1.73390	-5.26827	-0.75924
C	-0.31726	3.85749	-0.71826
H	3.75044	0.60885	-1.38155
C	-0.77127	2.52257	-0.67389
H	1.99869	2.07996	-0.42154
H	1.52497	-6.09171	-0.06641
C	1.46080	-3.95172	-0.37386
H	0.18825	4.29054	0.15140
H	4.33418	-1.60911	-0.73103
H	-3.62330	0.91477	-0.35828
H	4.24169	2.68674	0.45166
C	2.13506	2.24259	0.65034
H	1.03238	-3.74683	0.61411
H	-2.40274	3.87398	0.86865
C	4.06435	-1.30965	0.28786
C	3.39705	2.59152	1.14403
C	2.71831	-1.03620	0.60686
C	-3.75591	0.28127	0.52580
H	-5.70726	1.11556	0.94549
C	1.03760	2.10169	1.52283
C	-4.94060	0.39772	1.26704
H	6.09883	-1.43783	1.01975
C	-2.74324	-0.60315	0.93134
C	5.05361	-1.22760	1.27666
C	-2.54962	3.30780	1.79334
C	-1.79636	2.14551	2.03808
C	2.37339	-0.73816	1.93748
H	1.32216	-0.56035	2.18775
C	3.58062	2.80858	2.51791
H	-4.10468	4.62956	2.51794
H	4.57025	3.07347	2.90752
C	-3.51522	3.72751	2.72036
C	-5.15690	-0.36935	2.42823
C	-2.97261	-1.41461	2.05600
C	4.70504	-0.89747	2.59680
C	1.22177	2.34016	2.89822
C	3.36235	-0.66557	2.92765
H	-2.21899	-2.14699	2.37357
C	2.48801	2.69049	3.38978
C	-4.16051	-1.29231	2.79656
C	-2.01991	1.41209	3.22050
H	5.48027	-0.83465	3.36979

H	0.37661	2.25697	3.58849
H	-1.46680	0.48392	3.39590
H	3.08125	-0.41879	3.95722
C	-3.73799	2.99093	3.89288
H	-4.31080	-1.92447	3.68219
C	-2.98530	1.83280	4.14186
H	2.61867	2.87458	4.46290
H	-4.50489	3.31100	4.60840
H	-3.16648	1.23819	5.04437
C	-6.40239	-0.17644	3.26067
H	-7.31224	-0.14223	2.63349
H	-6.52918	-0.98565	4.00133
H	-6.35926	0.78125	3.81739

E(DMF)= -2768.637530316434; G= 0.58586449

Pd(PPh₃)₂(PhIF) (10e)

Pd	-0.85604	-0.70857	0.14816
P	-0.55306	1.49782	0.83897
P	1.37068	-1.17004	-0.64003
H	-1.30018	4.67511	-3.90209
H	2.44167	2.19265	-5.18393
H	0.34732	0.82604	-5.02660
H	2.84559	-4.67844	-3.93235
H	-2.11467	2.30730	-3.81674
C	2.27093	1.54371	-4.31673
C	1.09776	0.77805	-4.22851
C	-1.15298	4.07393	-2.99674
C	-1.61149	2.74960	-2.94907
C	2.46531	-4.47309	-2.92469
H	2.38041	-2.33032	-3.24473
H	2.44617	-6.56050	-2.33378
H	4.14505	2.06675	-3.35202
C	3.22406	1.47456	-3.28985
C	0.86917	-0.03802	-3.11391
H	-0.05406	-0.62510	-3.03775
C	2.20474	-3.14825	-2.53869
H	-0.13764	5.66269	-1.91615
C	2.24148	-5.52736	-2.02896
C	-0.50054	4.62886	-1.88338
C	-1.41660	1.97765	-1.79521
H	-1.74931	0.93356	-1.76329
C	3.00719	0.64592	-2.17804
C	1.82359	-0.10901	-2.07579
I	-1.88538	-2.66878	-1.35880
C	1.71273	-2.87706	-1.25118
C	1.75019	-5.25719	-0.74057
C	-0.30871	3.86218	-0.72581
H	3.75703	0.60258	-1.38275
C	-0.76692	2.52905	-0.67437
H	2.00741	2.08774	-0.42752
H	1.56238	-6.07802	-0.03865
C	1.48241	-3.93982	-0.35459
H	0.20477	4.29613	0.13868
H	4.32915	-1.60252	-0.72374
H	-3.61709	0.94423	-0.32540
H	4.25282	2.69105	0.44150
C	2.14597	2.24992	0.64410
H	1.07968	-3.73178	0.64351
H	-2.38344	3.88937	0.87900
C	4.05967	-1.30327	0.29529
C	3.40941	2.59686	1.13549
C	2.71391	-1.02859	0.61475
C	-3.75931	0.28565	0.53827
H	-5.75729	1.07142	0.95101
C	1.05022	2.11032	1.51885
C	-4.96895	0.37077	1.24721
H	6.09401	-1.43405	1.02675
C	-2.74473	-0.59880	0.94041
C	5.04911	-1.22293	1.28399

C	-2.53156	3.32003	1.80164
C	-1.78197	2.15485	2.04176
C	2.36942	-0.73181	1.94570
H	1.31843	-0.55403	2.19667
C	3.59586	2.81315	2.50909
H	-4.08130	4.64449	2.53375
H	4.58662	3.07646	2.89686
C	-3.49430	3.73998	2.73211
C	-5.15919	-0.44789	2.36392
C	-2.98087	-1.43744	2.04634
C	4.70107	-0.89339	2.60441
C	1.23704	2.34868	2.89395
C	3.35865	-0.66073	2.93571
H	-2.22100	-2.16336	2.36232
C	2.50474	2.69691	3.38308
C	-4.18374	-1.36414	2.76883
C	-2.00637	1.41744	3.22180
H	5.47646	-0.83193	3.37732
H	0.39317	2.26647	3.58586
H	-1.45543	0.48681	3.39270
H	3.07791	-0.41497	3.96563
C	-3.71722	3.00059	3.90246
H	-4.37149	-2.00794	3.63556
C	-2.96788	1.83882	4.14695
H	2.63773	2.88083	4.45590
H	-4.48299	3.31961	4.61940
H	-3.14877	1.24351	5.04911
F	-6.31331	-0.35632	3.06488

E(DMF)= -2828.596015810687; G= 0.55054845

Pd(PPh₃)₂(PhICl) (10f)

Pd	-0.85658	-0.71717	0.13952
P	-0.55063	1.49350	0.83698
P	1.37065	-1.17405	-0.64941
H	-1.27807	4.67717	-3.90218
H	2.43855	2.19468	-5.18910
H	0.35086	0.81721	-5.03839
H	2.86188	-4.67537	-3.94162
H	-2.09727	2.31097	-3.82205
C	2.26852	1.54475	-4.32251
C	1.09906	0.77301	-4.23798
C	-1.13340	4.07424	-2.99760
C	-1.59459	2.75077	-2.95286
C	2.47514	-4.47225	-2.93598
H	2.39432	-2.32856	-3.25103
H	2.45069	-6.56109	-2.35035
H	4.13728	2.07675	-3.35240
C	3.21896	1.48014	-3.29293
C	0.87114	-0.04404	-3.12406
H	-0.04979	-0.63506	-3.05042
C	2.21305	-3.14818	-2.54836
H	-0.11785	5.65972	-1.91240
C	2.24471	-5.52857	-2.04432
C	-0.48212	4.62631	-1.88210
C	-1.40311	1.97662	-1.79988
H	-1.73863	0.93335	-1.76972
C	3.00317	0.65001	-2.18199
C	1.82284	-0.11042	-2.08313
I	-1.89257	-2.67791	-1.35778
C	1.71293	-2.87987	-1.26330
C	1.74513	-5.26132	-0.75852
C	-0.29395	3.85754	-0.72535
H	3.75192	0.60891	-1.38557
C	-0.75395	2.52490	-0.67734
H	2.02024	2.07791	-0.41117
H	1.55219	-6.08376	-0.05990
C	1.47571	-3.94472	-0.37097
H	0.21720	4.28950	0.14148
H	4.33016	-1.60095	-0.73097

H	-3.62493	0.92279	-0.32870
H	4.26012	2.67872	0.47506
C	2.15124	2.23960	0.66151
H	1.06666	-3.73892	0.62501
H	-2.40602	3.86603	0.83954
C	4.05867	-1.30560	0.28867
C	3.41127	2.58524	1.16247
C	2.71205	-1.03438	0.60721
C	-3.74953	0.28533	0.55345
H	-5.68771	1.15597	1.03109
C	1.04890	2.10132	1.52811
C	-4.92053	0.42775	1.31405
H	6.09223	-1.43504	1.02261
C	-2.73898	-0.61072	0.93942
C	5.04656	-1.22679	1.27908
C	-2.56266	3.29835	1.76176
C	-1.79295	2.15122	2.02627
C	2.36508	-0.74260	1.93872
H	1.31350	-0.56684	2.18883
C	3.58746	2.80118	2.53752
H	-4.16778	4.58340	2.44216
H	4.57554	3.06345	2.93276
C	-3.56218	3.69630	2.66244
C	-5.08584	-0.34748	2.46919
C	-2.96060	-1.42907	2.06346
C	4.69600	-0.90261	2.60015
C	1.22532	2.33937	2.90457
C	3.35269	-0.67353	2.93042
H	-2.21122	-2.17288	2.36281
C	2.48970	2.68605	3.40334
C	-4.12491	-1.29911	2.83783
C	-2.02814	1.41754	3.20671
H	5.47017	-0.84238	3.37436
H	0.37568	2.25923	3.58970
H	-1.46017	0.50124	3.39816
H	3.07008	-0.43169	3.96073
C	-3.80377	2.95296	3.82640
H	-4.27989	-1.91775	3.72814
C	-3.02838	1.81568	4.09991
H	2.61474	2.87000	4.47710
H	-4.60827	3.24348	4.51179
H	-3.22726	1.21449	4.99399
Cl	-6.49709	-0.09749	3.48711

E(DMF)= -3188.943771685913; G= 0.55037475

Pd(PPh₃)₂(PhICF₃) (**10g**)

Pd	-0.86060	-0.70185	0.14139
P	-0.54283	1.50601	0.83863
P	1.36513	-1.16508	-0.64868
H	-1.26053	4.70153	-3.89285
H	2.44965	2.20492	-5.18311
H	0.35288	0.84138	-5.03235
H	2.81685	-4.66976	-3.95485
H	-2.09486	2.34072	-3.81496
C	2.27611	1.55487	-4.31734
C	1.10155	0.79097	-4.23279
C	-1.11687	4.09588	-2.98996
C	-1.58651	2.77531	-2.94647
C	2.44082	-4.46567	-2.94537
H	2.36174	-2.32190	-3.25991
H	2.41728	-6.55441	-2.35946
H	4.14949	2.07265	-3.34840
C	3.22720	1.48226	-3.28886
C	0.86931	-0.02625	-3.11985
H	-0.05538	-0.61134	-3.04647
C	2.18591	-3.14094	-2.55525
H	-0.08821	5.67284	-1.90475
C	2.21700	-5.52139	-2.05135
C	-0.45873	4.64165	-1.87538

C	-1.39648	1.99773	-1.79560
H	-1.73893	0.95672	-1.76620
C	3.00703	0.65188	-2.17900
C	1.82167	-0.10069	-2.08008
I	-1.89691	-2.66257	-1.35773
C	1.69978	-2.87147	-1.26514
C	1.73156	-5.25290	-0.76041
C	-0.27203	3.86956	-0.72061
H	3.75663	0.60436	-1.38376
C	-0.74033	2.53979	-0.67407
H	2.03381	2.07901	-0.40268
H	1.54409	-6.07482	-0.05972
C	1.46966	-3.93564	-0.37011
H	0.24360	4.29678	0.14588
H	4.32213	-1.60454	-0.72755
H	-3.62128	0.94720	-0.32281
H	4.27441	2.66793	0.49038
C	2.16311	2.23774	0.67063
H	1.07226	-3.72885	0.63037
H	-2.39522	3.87868	0.83831
C	4.05042	-1.31185	0.29278
C	3.42341	2.57683	1.17541
C	2.70470	-1.03511	0.61039
C	-3.75671	0.29369	0.54558
H	-5.71192	1.12070	0.98525
C	1.05827	2.10263	1.53441
C	-4.94445	0.39888	1.28330
H	6.08195	-1.45511	1.02958
C	-2.74370	-0.59847	0.93483
C	5.03697	-1.24255	1.28522
C	-2.55461	3.30989	1.75939
C	-1.78540	2.16322	2.02578
C	2.35688	-0.74763	1.94263
H	1.30583	-0.56750	2.19187
C	3.59699	2.78938	2.55129
H	-4.16253	4.59330	2.43666
H	4.58524	3.04640	2.94951
C	-3.55687	3.70648	2.65788
C	-5.14459	-0.40533	2.41674
C	-2.97598	-1.43960	2.04232
C	4.68580	-0.92269	2.60715
C	1.23191	2.33780	2.91171
C	3.34314	-0.68822	2.93628
H	-2.22189	-2.17827	2.34123
C	2.49657	2.67789	3.41420
C	-4.16031	-1.34148	2.78322
C	-2.02429	1.42742	3.20451
H	5.45894	-0.87012	3.38292
H	0.38012	2.26084	3.59447
H	-1.45742	0.51009	3.39588
H	3.06005	-0.44987	3.96727
C	-3.80068	2.96248	3.82065
H	-4.32039	-1.99086	3.65135
C	-3.02600	1.82486	4.09565
H	2.61976	2.85954	4.48855
H	-4.60803	3.25000	4.50349
H	-3.23044	1.22322	4.98739
C	-6.36090	-0.23077	3.28675
F	-7.37336	0.40568	2.65208
F	-6.84525	-1.41439	3.73698
F	-6.07746	0.50983	4.40290

E(DMF)= -3066.423573130381; G= 0.56206249

Pd(PPh₃)₂(PhICN) (**10h**)

Pd	-0.85668	-0.71439	0.14518
P	-0.54723	1.49765	0.83937
P	1.36957	-1.16954	-0.64620
H	-1.28115	4.68952	-3.89152
H	2.42193	2.18838	-5.19685

H	0.33724	0.80724	-5.03866
H	2.82198	-4.68196	-3.94305
H	-2.09142	2.32032	-3.81979
C	2.25441	1.54105	-4.32788
C	1.08658	0.76741	-4.23910
C	-1.13497	4.08440	-2.98871
C	-1.59139	2.75913	-2.94863
C	2.45009	-4.47499	-2.93263
H	2.35874	-2.33320	-3.25689
H	2.44020	-6.56097	-2.33684
H	4.12385	2.07937	-3.36273
C	3.20667	1.48147	-3.29969
C	0.86200	-0.04640	-3.12214
H	-0.05762	-0.63903	-3.04561
C	2.19060	-3.14972	-2.54747
H	-0.12613	5.67036	-1.89804
C	2.23628	-5.52757	-2.03253
C	-0.48664	4.63558	-1.87101
C	-1.39842	1.98239	-1.79766
H	-1.73035	0.93795	-1.77097
C	2.99443	0.65441	-2.18584
C	1.81561	-0.10777	-2.08266
I	-1.88757	-2.68606	-1.34128
C	1.71011	-2.87673	-1.25600
C	1.75647	-5.25550	-0.74024
C	-0.29656	3.86421	-0.71641
H	3.74522	0.61654	-1.39119
C	-0.75242	2.52990	-0.67293
H	2.02140	2.07862	-0.40928
H	1.57716	-6.07505	-0.03466
C	1.49031	-3.93773	-0.35459
H	0.21257	4.29513	0.15212
H	4.32770	-1.58681	-0.73067
H	-3.61703	0.91412	-0.34521
H	4.26159	2.68217	0.47464
C	2.15328	2.24154	0.66312
H	1.09795	-3.72836	0.64736
H	-2.41963	3.85469	0.84187
C	4.05656	-1.29354	0.28964
C	3.41330	2.58893	1.16270
C	2.70961	-1.02624	0.61027
C	-3.75314	0.27498	0.53360
H	-5.69919	1.12552	0.97613
C	1.05195	2.10370	1.53105
C	-4.93262	0.40179	1.27395
H	6.09112	-1.41902	1.02121
C	-2.73944	-0.61521	0.93390
C	5.04523	-1.21389	1.27914
C	-2.56737	3.28980	1.76728
C	-1.79047	2.14728	2.03067
C	2.36320	-0.73783	1.94263
H	1.31159	-0.56513	2.19462
C	3.58999	2.80737	2.53730
H	-4.17029	4.57270	2.45743
H	4.57803	3.07130	2.93144
C	-3.55969	3.68860	2.67549
C	-5.13103	-0.38154	2.43415
C	-2.97118	-1.44178	2.05344
C	4.69519	-0.89311	2.60116
C	1.22853	2.34452	2.90690
C	3.35166	-0.66819	2.93339
H	-2.21733	-2.17801	2.35878
C	2.49297	2.69329	3.40409
C	-4.14571	-1.32657	2.80395
C	-2.01442	1.41578	3.21483
H	5.46995	-0.83240	3.37468
H	0.37959	2.26555	3.59289
H	-1.44086	0.50239	3.40523
H	3.06957	-0.42933	3.96452
C	-3.78534	2.95204	3.84719
H	-4.30383	-1.95411	3.68822
C	-3.00500	1.81711	4.11781
H	2.61845	2.87979	4.47730

H	-4.57902	3.24841	4.54274
H	-3.18841	1.22431	5.02091
C	-6.29954	-0.19598	3.24241
N	-7.24840	-0.03216	3.91098

E(DMF)= -2821.569135567697; G= 0.55809508

Pd(PPh₃)₂(PhINO₂) (**10i**)

Pd	-0.87343	-0.94204	0.21167
P	-0.12464	0.74327	1.66701
P	1.24494	-1.51449	-0.76786
H	0.76462	5.30739	-1.72120
H	2.62414	2.84930	-4.24681
H	0.66815	1.35697	-4.73579
H	2.58203	-4.33458	-4.70795
H	-0.53242	3.33407	-2.55918
C	2.40058	2.00028	-3.59001
C	1.30454	1.16585	-3.86373
C	0.59212	4.44343	-1.06829
C	-0.13625	3.34161	-1.53862
C	2.05536	-4.29959	-3.74720
H	2.45829	-2.19047	-3.44499
H	1.50774	-6.39934	-3.78739
H	4.06197	2.39112	-2.24994
C	3.20459	1.74437	-2.47077
C	1.00374	0.09384	-3.01577
H	0.12721	-0.53590	-3.21245
C	1.98421	-3.08969	-3.03850
H	1.67596	5.29704	0.61049
C	1.45366	-5.45609	-3.23093
C	1.10713	4.43650	0.23855
C	-0.34531	2.23065	-0.70954
H	-0.89662	1.35855	-1.08196
C	2.91957	0.65822	-1.62832
C	1.81358	-0.17261	-1.88863
I	-2.21630	-2.02293	-1.83760
C	1.29796	-3.03341	-1.81292
C	0.77524	-5.40284	-2.00224
C	0.89910	3.32898	1.07125
H	3.56550	0.45902	-0.76968
C	0.17352	2.21457	0.59925
H	2.67091	1.16375	0.93232
H	0.29580	-6.30200	-1.59859
C	0.69203	-4.19615	-1.29784
H	1.30753	3.32536	2.08708
H	4.22433	-1.81985	-1.08285
H	-3.07074	1.37211	0.20979
H	4.82841	0.87663	2.13370
C	2.67185	0.84980	1.97792
H	0.14414	-4.14883	-0.34991
H	-1.39009	3.39402	2.29254
C	3.95831	-2.04423	-0.04409
C	3.88386	0.69768	2.65985
C	2.62057	-1.93232	0.38245
C	-3.45798	0.56313	0.83916
H	-5.15442	1.74009	1.54232
C	1.44513	0.61631	2.63132
C	-4.62575	0.78406	1.57485
H	5.99010	-2.54189	0.51901
C	-2.74817	-0.64898	0.95639
C	4.94898	-2.46333	0.85437
C	-1.79969	2.64542	2.97676
C	-1.34343	1.31521	2.92574
C	2.28260	-2.28958	1.70118
H	1.23807	-2.21170	2.02365
C	3.88848	0.30166	4.00576
H	-3.17997	4.04138	3.88905
H	4.83783	0.17274	4.53859
C	-2.81648	3.00711	3.87280
C	-5.09978	-0.23146	2.41775

C	-3.29965	-1.68665	1.73892
C	4.60777	-2.80156	2.17410
C	1.45554	0.22693	3.98469
C	3.27138	-2.72541	2.59272
H	-2.79837	-2.66055	1.79442
C	2.67213	0.06979	4.66493
C	-4.46885	-1.48304	2.47870
C	-1.91116	0.35795	3.79124
H	5.38441	-3.13041	2.87439
H	0.51546	0.05623	4.51724
H	-1.60013	-0.68964	3.72470
H	2.99817	-2.99013	3.61963
C	-3.38847	2.04842	4.72036
H	-4.88490	-2.26127	3.12423
C	-2.92703	0.72322	4.68250
H	2.66583	-0.23269	5.71852
H	-4.21167	2.32417	5.38937
H	-3.38996	-0.03871	5.31928
N	-6.24100	0.04588	3.30770
O	-6.61428	-0.85221	4.06160
O	-6.73932	1.17055	3.26882

E(DMF)= -2933.842451004486; G= 0.56197834

$[\text{Pd}(\text{PPh}_3)(\text{CO})(\text{PhINH}_2)]^\ddagger$ (**11bTS**)

Pd	0.38190	1.24842	0.52306
P	-1.32232	-0.43190	0.45528
C	-0.79786	-2.05696	-0.23909
C	-1.46875	-2.70171	-1.29569
C	0.34122	-2.66546	0.32961
C	-1.00468	-3.93742	-1.77478
H	-2.35486	-2.24011	-1.74351
C	0.79423	-3.90254	-0.14369
H	0.87187	-2.16261	1.14713
C	0.12353	-4.54131	-1.20054
H	-1.53190	-4.43078	-2.60016
H	1.68002	-4.36547	0.30641
H	0.48252	-5.50616	-1.57607
C	-2.76585	0.03166	-0.58778
C	-2.48481	0.60185	-1.84767
C	-4.10333	-0.08888	-0.16987
C	-3.52506	1.03030	-2.67838
H	-1.44178	0.73322	-2.16010
C	-5.14445	0.35370	-1.00172
H	-4.33514	-0.51518	0.81126
C	-4.85891	0.91193	-2.25566
H	-3.29478	1.48919	-3.64578
H	-6.18409	0.26274	-0.66307
H	-5.67120	1.26843	-2.89966
C	-2.07073	-0.94021	2.06462
C	-1.94532	-0.08415	3.17584
C	-2.76895	-2.15795	2.20340
C	-2.53254	-0.42867	4.40273
H	-1.36701	0.84256	3.08393
C	-3.35102	-2.50089	3.43177
H	-2.85043	-2.83825	1.34782
C	-3.23852	-1.63432	4.53185
H	-2.42731	0.24447	5.26203
H	-3.89029	-3.45046	3.53252
H	-3.69293	-1.90510	5.49219
C	-2.89642	4.01294	-1.24400
C	-1.51483	4.13943	-1.49576
C	-3.30378	3.38757	-0.03533
H	-1.17104	4.64607	-2.40625
H	-4.37377	3.26666	0.17453
C	-0.56712	3.65806	-0.57850
C	-2.37258	2.88379	0.86598
H	0.49910	3.83663	-0.75698
H	-2.71749	2.39220	1.78058
C	-0.99070	2.96173	0.57661

I	0.46922	3.24693	2.45842
C	2.04831	0.41377	-0.03562
O	2.92398	-0.20718	-0.46591
N	-3.84096	4.44793	-2.16716
H	-3.53393	5.17189	-2.81150
H	-4.77173	4.62287	-1.79991

E(DMF)= -1861.972028619451; G= 0.32306057

$[\text{Pd}(\text{PPh}_3)(\text{CO})(\text{PhIOH})]^\ddagger$ (**11cTS**)

Pd	0.41633	1.25674	0.51005
P	-1.31255	-0.39214	0.42021
C	-0.81264	-2.02734	-0.26974
C	-1.46463	-2.64480	-1.35403
C	0.29124	-2.67049	0.32969
C	-1.01593	-3.88699	-1.83102
H	-2.32485	-2.15816	-1.82539
C	0.72919	-3.91325	-0.14263
H	0.80600	-2.19187	1.17132
C	0.07815	-4.52430	-1.22788
H	-1.52863	-4.35878	-2.67776
H	1.58759	-4.40300	0.33165
H	0.42544	-5.49392	-1.60204
C	-2.74536	0.09287	-0.62705
C	-2.45096	0.63321	-1.89696
C	-4.08585	0.01299	-0.20831
C	-3.48168	1.06864	-2.73681
H	-1.40521	0.72849	-2.21343
C	-5.11541	0.46725	-1.04748
H	-4.32811	-0.38822	0.78071
C	-4.81758	0.99434	-2.31182
H	-3.23954	1.49293	-3.71803
H	-6.15643	0.41382	-0.70580
H	-5.62178	1.36188	-2.95900
C	-2.05889	-0.88796	2.03358
C	-1.85039	-0.07403	3.16353
C	-2.82440	-2.06611	2.15957
C	-2.42239	-0.41845	4.39772
H	-1.22069	0.81946	3.07788
C	-3.39228	-2.40868	3.39438
H	-2.96717	-2.71755	1.28958
C	-3.19673	-1.58253	4.51391
H	-2.25239	0.22159	5.27160
H	-3.98424	-3.32738	3.48567
H	-3.64007	-1.85347	5.47928
C	-2.94923	3.94683	-1.12880
C	-1.59271	4.08001	-1.46201
C	-3.30916	3.36895	0.11019
H	-1.30181	4.55787	-2.40702
H	-4.37123	3.26497	0.35451
C	-0.59474	3.64012	-0.57299
C	-2.33005	2.90463	0.98154
H	0.45979	3.81940	-0.80959
H	-2.62516	2.44023	1.92715
C	-0.96251	2.98783	0.62504
I	0.57334	3.28413	2.41555
C	2.09716	0.36860	0.09900
O	3.01133	-0.32111	-0.06064
O	-3.95870	4.36290	-1.94642
H	-3.56991	4.73817	-2.75131

E(DMF)= -1881.850577337497; G= 0.31155776

$[\text{Pd}(\text{PPh}_3)(\text{CO})(\text{PhICH}_3)]^\ddagger$ (**11dTS**)

Pd	0.41384	1.24842	0.50567
P	-1.31774	-0.39186	0.42604

C	-0.81344	-2.03220	-0.25132
C	-1.49051	-2.67916	-1.30269
C	0.31226	-2.65292	0.33032
C	-1.04533	-3.92839	-1.76417
H	-2.36690	-2.20979	-1.76125
C	0.74724	-3.90275	-0.12639
H	0.84695	-2.15023	1.14525
C	0.07063	-4.54346	-1.17821
H	-1.57774	-4.42321	-2.58533
H	1.62336	-4.37461	0.33328
H	0.41525	-5.51852	-1.54057
C	-2.74143	0.07840	-0.64007
C	-2.43469	0.59427	-1.91678
C	-4.08670	-0.01418	-0.23984
C	-3.45866	0.98330	-2.78732
H	-1.38564	0.70233	-2.21764
C	-5.11082	0.38997	-1.11050
H	-4.33674	-0.39529	0.75525
C	-4.80083	0.88188	-2.38666
H	-3.20771	1.38528	-3.77550
H	-6.15675	0.31839	-0.78766
H	-5.60246	1.19551	-3.06572
C	-2.07371	-0.88084	2.03724
C	-1.86806	-0.06297	3.16484
C	-2.83668	-2.06025	2.16664
C	-2.43970	-0.40452	4.39980
H	-1.23980	0.83105	3.07794
C	-3.40477	-2.39976	3.40224
H	-2.97606	-2.71616	1.29950
C	-3.21152	-1.56983	4.51937
H	-2.27058	0.23872	5.27152
H	-3.99421	-3.31975	3.49630
H	-3.65415	-1.83894	5.48555
C	-2.89489	3.97081	-1.16845
C	-1.52549	4.07216	-1.45730
C	-3.26911	3.38288	0.06459
H	-1.20054	4.54283	-2.39404
H	-4.33372	3.27697	0.30830
C	-0.54593	3.62525	-0.54942
C	-2.32314	2.90526	0.96828
H	0.51570	3.79643	-0.76040
H	-2.64396	2.43822	1.90408
C	-0.94941	2.98365	0.64280
I	0.55653	3.24224	2.45222
C	2.07834	0.39483	-0.01900
O	2.97313	-0.25536	-0.35485
C	-3.94312	4.50999	-2.10988
H	-3.53595	4.67153	-3.12258
H	-4.80064	3.81911	-2.19033
H	-4.33819	5.48052	-1.75206

E(DMF)= -1845.917982782079; G= 0.33322334

[Pd(PPh₃)(CO)(PhIF)][‡] (**11eTS**)

Pd	0.41383	1.25328	0.51427
P	-1.31135	-0.39941	0.41985
C	-0.80117	-2.03811	-0.25384
C	-1.46735	-2.68132	-1.31426
C	0.31672	-2.66153	0.33985
C	-1.01924	-3.93060	-1.77276
H	-2.33778	-2.20911	-1.78142
C	0.75428	-3.91149	-0.11391
H	0.84250	-2.16182	1.16240
C	0.08850	-4.54890	-1.17467
H	-1.54295	-4.42291	-2.60090
H	1.62355	-4.38641	0.35551
H	0.43505	-5.52424	-1.53432
C	-2.73526	0.07534	-0.64363
C	-2.43058	0.59608	-1.91929
C	-4.07857	0.00858	-0.23120

C	-3.45332	1.02879	-2.77055
H	-1.38257	0.68041	-2.23159
C	-5.10069	0.45646	-1.08307
H	-4.32853	-0.37861	0.76147
C	-4.79220	0.96666	-2.35206
H	-3.20351	1.44306	-3.75367
H	-6.14417	0.41117	-0.74768
H	-5.59014	1.32905	-3.00995
C	-2.06899	-0.88509	2.03098
C	-1.86103	-0.06914	3.15950
C	-2.84221	-2.05819	2.15677
C	-2.44122	-0.40592	4.39194
H	-1.22543	0.82015	3.07465
C	-3.41875	-2.39292	3.38969
H	-2.98415	-2.71209	1.28848
C	-3.22376	-1.56447	4.50764
H	-2.27120	0.23568	5.26467
H	-4.01686	-3.30760	3.48088
H	-3.67376	-1.82945	5.47155
C	-2.89742	3.87568	-1.16125
C	-1.55127	4.02746	-1.49211
C	-3.29642	3.32914	0.07000
H	-1.27401	4.48962	-2.44528
H	-4.36340	3.22090	0.28882
C	-0.56808	3.61472	-0.57297
C	-2.32816	2.89178	0.97161
H	0.48945	3.80039	-0.78975
H	-2.63429	2.44007	1.91956
C	-0.95751	2.98209	0.63180
I	0.55935	3.27564	2.42590
C	2.08112	0.39571	-0.00145
O	2.97472	-0.25844	-0.33127
F	-3.84423	4.27310	-2.03592

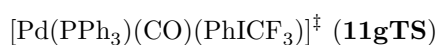
E(DMF)= -1905.873931422175; G= 0.29943669

[Pd(PPh₃)(CO)(PhICl)][‡] (**11fTS**)

Pd	0.40704	1.24694	0.50139
P	-1.31431	-0.40575	0.42394
C	-0.80377	-2.04100	-0.25831
C	-1.47932	-2.68355	-1.31331
C	0.32083	-2.66367	0.32324
C	-1.03316	-3.93085	-1.77894
H	-2.35547	-2.21247	-1.77060
C	0.75667	-3.91164	-0.13776
H	0.85328	-2.16536	1.14223
C	0.08188	-4.54800	-1.19338
H	-1.56428	-4.42258	-2.60271
H	1.63158	-4.38564	0.32195
H	0.42694	-5.52175	-1.55872
C	-2.74560	0.06685	-0.62845
C	-2.45167	0.58448	-1.90811
C	-4.08516	-0.00462	-0.20561
C	-3.48228	1.00581	-2.75462
H	-1.40613	0.67340	-2.22764
C	-5.11540	0.43442	-1.05257
H	-4.32601	-0.38967	0.79023
C	-4.81803	0.93795	-2.32650
H	-3.24236	1.42011	-3.73984
H	-6.15625	0.38672	-0.70947
H	-5.62153	1.29583	-2.97973
C	-2.06327	-0.89672	2.03741
C	-1.88260	-0.06475	3.15887
C	-2.80956	-2.08634	2.17013
C	-2.46171	-0.40335	4.39121
H	-1.26821	0.83859	3.06972
C	-3.38472	-2.42309	3.40321
H	-2.93240	-2.75059	1.30691
C	-3.21611	-1.57971	4.51420
H	-2.31252	0.25087	5.25843

H	-3.96163	-3.35068	3.49971
H	-3.66485	-1.84630	5.47824
C	-2.86403	3.93984	-1.20299
C	-1.50353	4.07164	-1.49915
C	-3.28667	3.36452	0.01255
H	-1.18754	4.54629	-2.43354
H	-4.35571	3.25731	0.21939
C	-0.54486	3.63228	-0.56796
C	-2.34247	2.90282	0.92653
H	0.51842	3.81256	-0.76106
H	-2.67436	2.43875	1.85993
C	-0.96260	2.99025	0.62286
I	0.50542	3.26345	2.43536
C	2.09064	0.39530	0.02971
O	2.99592	-0.27213	-0.23551
Cl	-4.05984	4.51599	-2.34296

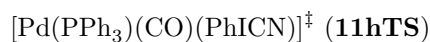
E(DMF)= -2266.222364614419; G= 0.29728792



Pd	0.45199	1.19976	0.50305
P	-1.30042	-0.40031	0.39170
C	-0.80385	-2.05320	-0.25892
C	-1.45643	-2.68964	-1.33165
C	0.28653	-2.69462	0.36589
C	-1.02071	-3.94950	-1.77291
H	-2.30617	-2.20409	-1.82247
C	0.71187	-3.95458	-0.07144
H	0.80054	-2.20219	1.20002
C	0.06070	-4.58487	-1.14546
H	-1.53340	-4.43615	-2.61113
H	1.56011	-4.44341	0.42172
H	0.39801	-5.56811	-1.49217
C	-2.70673	0.08077	-0.68562
C	-2.38235	0.56376	-1.97106
C	-4.05529	0.03166	-0.28680
C	-3.39296	0.96816	-2.85009
H	-1.32991	0.63290	-2.27226
C	-5.06424	0.45212	-1.16663
H	-4.31781	-0.32440	0.71428
C	-4.73710	0.91762	-2.44805
H	-3.13063	1.35246	-3.84132
H	-6.11206	0.42400	-0.84391
H	-5.52477	1.26333	-3.12631
C	-2.05678	-0.85680	2.01072
C	-1.80261	-0.05406	3.13925
C	-2.86413	-2.00574	2.14466
C	-2.36875	-0.38004	4.38101
H	-1.14229	0.81619	3.04557
C	-3.42784	-2.32891	3.38641
H	-3.04119	-2.65147	1.27671
C	-3.18486	-1.51422	4.50508
H	-2.16167	0.25026	5.25383
H	-4.05246	-3.22497	3.48435
H	-3.62379	-1.77146	5.47608
C	-2.98351	3.91322	-1.12223
C	-1.63340	4.02715	-1.49044
C	-3.31853	3.35109	0.12701
H	-1.36252	4.47427	-2.45283
H	-4.36923	3.24618	0.41262
C	-0.61981	3.60587	-0.61853
C	-2.32415	2.90576	0.99550
H	0.43124	3.76219	-0.88517
H	-2.59895	2.46104	1.95612
C	-0.96634	2.99918	0.61350
I	0.58960	3.32693	2.33044
C	2.12641	0.31436	0.07418
O	3.01091	-0.38883	-0.16717
C	-4.04478	4.47908	-2.03057
F	-4.07558	5.83675	-1.97817

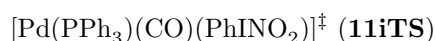
F	-3.82663	4.15487	-3.33330
F	-5.28818	4.04642	-1.71215

E(DMF)= -2143.701393007304; G= 0.31027288



Pd	0.43256	1.22335	0.53568
P	-1.31077	-0.38838	0.39455
C	-0.79341	-2.03007	-0.26603
C	-1.42434	-2.65694	-1.35707
C	0.29144	-2.67144	0.36830
C	-0.97249	-3.90794	-1.80718
H	-2.26990	-2.17107	-1.85476
C	0.73281	-3.92259	-0.07818
H	0.78798	-2.18660	1.21738
C	0.10339	-4.54347	-1.17050
H	-1.46822	-4.38734	-2.65952
H	1.57622	-4.41204	0.42254
H	0.45318	-5.51986	-1.52396
C	-2.71540	0.09339	-0.68442
C	-2.39110	0.58697	-1.96633
C	-4.06387	0.04505	-0.28527
C	-3.40149	1.00788	-2.83789
H	-1.33901	0.65447	-2.26884
C	-5.07229	0.48249	-1.15811
H	-4.32722	-0.31880	0.71270
C	-4.74556	0.96375	-2.43372
H	-3.13995	1.40244	-3.82605
H	-6.11957	0.45656	-0.83342
H	-5.52999	1.33241	-3.10289
C	-2.06654	-0.86204	2.00832
C	-1.80400	-0.08017	3.14953
C	-2.88192	-2.00722	2.12491
C	-2.37063	-0.42224	4.38677
H	-1.13760	0.78687	3.06917
C	-3.44639	-2.34625	3.36197
H	-3.06490	-2.63744	1.24683
C	-3.19563	-1.55170	4.49334
H	-2.15770	0.19191	5.26957
H	-4.07784	-3.23887	3.44619
H	-3.63557	-1.82110	5.46054
C	-3.07064	3.82812	-1.06278
C	-1.72013	3.98730	-1.44421
C	-3.36920	3.28204	0.21416
H	-1.48065	4.42610	-2.41851
H	-4.41406	3.14993	0.51131
C	-0.68704	3.61506	-0.57727
C	-2.35063	2.89139	1.07416
H	0.35502	3.80126	-0.85852
H	-2.59678	2.46005	2.04854
C	-0.99886	3.00780	0.66630
I	0.57046	3.36636	2.34524
C	2.09427	0.33562	0.05521
O	2.95478	-0.35901	-0.27774
C	-4.12439	4.20719	-1.95186
N	-4.98887	4.50122	-2.68738

E(DMF)= -1898.846627951669; G= 0.30572353



Pd	0.49785	1.21638	0.49843
P	-1.27457	-0.35177	0.35213
C	-0.77706	-2.01966	-0.25632
C	-1.43730	-2.68438	-1.30692
C	0.31094	-2.64698	0.38558
C	-1.01077	-3.95997	-1.70964

H	-2.28443	-2.20726	-1.81047
C	0.72766	-3.92238	-0.01383
H	0.83016	-2.13049	1.20210
C	0.06915	-4.58146	-1.06575
H	-1.52845	-4.46938	-2.53110
H	1.57476	-4.40095	0.49116
H	0.40017	-5.57658	-1.38337
C	-2.61327	0.15178	-0.79672
C	-2.21286	0.57340	-2.08342
C	-3.97658	0.19648	-0.44999
C	-3.16442	1.00943	-3.01294
H	-1.14758	0.57082	-2.34497
C	-4.92495	0.64574	-1.38115
H	-4.29883	-0.10166	0.55215
C	-4.52335	1.04732	-2.66287
H	-2.84379	1.35016	-4.00341
H	-5.98135	0.70468	-1.09630
H	-5.26265	1.42867	-3.37527
C	-2.09028	-0.78033	1.94819
C	-1.73441	-0.07848	3.11566
C	-3.02410	-1.83422	2.03087
C	-2.32607	-0.40454	4.34552
H	-0.97610	0.71186	3.06051
C	-3.61518	-2.15603	3.25979
H	-3.27795	-2.41041	1.13350
C	-3.27110	-1.43840	4.41763
H	-2.04060	0.14688	5.24879
H	-4.34065	-2.97650	3.31720
H	-3.73224	-1.69486	5.37841
C	-3.12482	3.69859	-0.83881
C	-1.83332	3.87426	-1.35432
C	-3.32757	3.22526	0.47383
H	-1.71456	4.26238	-2.36877
H	-4.34906	3.10675	0.84304
C	-0.72475	3.57613	-0.55636
C	-2.23390	2.90096	1.26552
H	0.28612	3.77011	-0.92992
H	-2.38751	2.52052	2.27884
C	-0.92113	3.01998	0.73723
I	0.76083	3.39641	2.24392
C	2.12061	0.32765	-0.09634
O	2.94209	-0.36332	-0.52202
N	-4.28337	4.01193	-1.67708
O	-5.40241	3.91669	-1.16983
O	-4.07622	4.33965	-2.84704

E(DMF)= -2011.122542897753; G= 0.31087996

Pd(PPh₃)(CO)(PhINH₂) (11b)

Pd	-1.01350	0.44272	0.09567
P	1.34596	-0.14824	0.03991
C	1.91856	-1.57589	-0.96758
C	2.20764	-2.82498	-0.38356
C	2.01179	-1.42725	-2.36879
C	2.58592	-3.90924	-1.18923
H	2.14805	-2.95431	0.70210
C	2.39377	-2.51419	-3.16602
H	1.78502	-0.46300	-2.83244
C	2.67901	-3.75766	-2.58072
H	2.81435	-4.87528	-0.72337
H	2.46431	-2.38615	-4.25279
H	2.97582	-4.60663	-3.20781
C	1.98615	-0.52609	1.72893
C	3.19459	-0.00119	2.22474
C	1.21454	-1.37527	2.55039
C	3.62519	-0.32648	3.52015
H	3.79790	0.66792	1.60243
C	1.65334	-1.70678	3.83899
H	0.26411	-1.77476	2.17771
C	2.85988	-1.18097	4.32744

H	4.56488	0.09181	3.89868
H	1.04559	-2.36864	4.46728
H	3.19820	-1.43230	5.33898
C	2.36627	1.25850	-0.54708
C	3.69150	1.07725	-0.99328
C	1.81279	2.55321	-0.52069
C	4.45333	2.18173	-1.39855
H	4.12217	0.07035	-1.03012
C	2.57944	3.65557	-0.92466
H	0.77312	2.68888	-0.19973
C	3.89947	3.47175	-1.36307
H	5.48167	2.03366	-1.74776
H	2.13884	4.65940	-0.90750
H	4.49541	4.33322	-1.68622
C	-1.15101	0.76044	1.95466
O	-1.28720	1.01826	3.06878
C	-5.76282	1.71448	0.13832
C	-4.75348	2.69213	-0.01840
C	-3.39809	2.33277	-0.02054
C	-3.01701	0.99045	0.12455
C	-4.00781	0.01271	0.29877
C	-5.36496	0.36706	0.30070
H	-5.03728	3.74424	-0.15360
H	-2.64186	3.11492	-0.15860
H	-3.73585	-1.04319	0.41937
H	-6.12950	-0.41155	0.42178
I	-1.23782	0.30503	-2.53408
N	-7.11228	2.06182	0.07787
H	-7.32511	3.02768	0.31218
H	-7.75280	1.41184	0.52480

E(DMF)= -1861.998993554512; G= 0.32735718

Pd(PPh₃)(CO)(PhIOH) (11c)

Pd	-1.00421	0.46946	0.09571
P	1.34969	-0.13822	0.03682
C	1.91224	-1.56139	-0.98037
C	2.17860	-2.81955	-0.40513
C	2.01829	-1.40107	-2.37928
C	2.54810	-3.90150	-1.21779
H	2.10751	-2.95748	0.67879
C	2.39208	-2.48576	-3.18337
H	1.80918	-0.42952	-2.83591
C	2.65491	-3.73827	-2.60702
H	2.75877	-4.87502	-0.75928
H	2.47332	-2.34905	-4.26829
H	2.94486	-4.58554	-3.23952
C	1.97709	-0.53642	1.72537
C	3.19865	-0.04507	2.22309
C	1.18352	-1.36949	2.54232
C	3.62062	-0.38740	3.51687
H	3.81882	0.61132	1.60386
C	1.61353	-1.71798	3.82951
H	0.22347	-1.74308	2.16741
C	2.83326	-1.22569	4.32011
H	4.57051	0.00503	3.89743
H	0.98900	-2.36689	4.45482
H	3.16490	-1.49026	5.33044
C	2.38065	1.26666	-0.53529
C	3.70544	1.08031	-0.98104
C	1.83644	2.56512	-0.49746
C	4.47589	2.18323	-1.37389
H	4.12891	0.07082	-1.02779
C	2.61182	3.66587	-0.88906
H	0.79750	2.70564	-0.17622
C	3.93139	3.47685	-1.32656
H	5.50378	2.03117	-1.72267
H	2.17873	4.67274	-0.86218
H	4.53431	4.33713	-1.63967
C	-1.09678	0.86997	1.94232

O	-1.20605	1.17740	3.04628
C	-5.74312	1.70559	0.14048
C	-4.76462	2.67716	-0.14158
C	-3.40303	2.33078	-0.14364
C	-3.00896	1.01276	0.12598
C	-3.98485	0.04736	0.42345
C	-5.34588	0.38563	0.42585
H	-5.06749	3.70859	-0.37088
H	-2.65893	3.09898	-0.38413
H	-3.69624	-0.98824	0.64042
H	-6.11503	-0.36373	0.64328
I	-1.26491	0.22300	-2.52130
O	-7.08012	1.98655	0.15311
H	-7.20077	2.91899	-0.08248

E(DMF)= -1881.878934130087; G= 0.31720914

Pd(PPh₃)(CO)(PhICH₃) (11d)

Pd	-1.00804	0.45967	0.10084
P	1.35011	-0.14402	0.04200
C	1.91512	-1.56769	-0.97365
C	2.19234	-2.82242	-0.39610
C	2.01088	-1.41170	-2.37380
C	2.56335	-3.90487	-1.20740
H	2.12900	-2.95726	0.68874
C	2.38601	-2.49686	-3.17664
H	1.79282	-0.44308	-2.83245
C	2.66036	-3.74577	-2.59784
H	2.78289	-4.87549	-0.74692
H	2.45932	-2.36331	-4.26252
H	2.95136	-4.59344	-3.22932
C	1.98353	-0.53608	1.72974
C	3.19756	-0.02794	2.22911
C	1.20149	-1.38155	2.54517
C	3.62323	-0.36571	3.52289
H	3.80885	0.63810	1.61136
C	1.63535	-1.72540	3.83226
H	0.24713	-1.76848	2.16915
C	2.84738	-1.21610	4.32455
H	4.56712	0.03981	3.90470
H	1.01970	-2.38403	4.45621
H	3.18195	-1.47706	5.33486
C	2.37459	1.26304	-0.53653
C	3.70148	1.08095	-0.97790
C	1.82297	2.55859	-0.50940
C	4.46665	2.18536	-1.37677
H	4.13075	0.07353	-1.01615
C	2.59299	3.66090	-0.90724
H	0.78239	2.69562	-0.19190
C	3.91465	3.47618	-1.34016
H	5.49626	2.03667	-1.72190
H	2.15400	4.66540	-0.88900
H	4.51339	4.33758	-1.65819
C	-1.09562	0.85222	1.95015
O	-1.19830	1.15369	3.05622
C	-5.75801	1.71093	0.12729
C	-4.75765	2.67869	-0.09064
C	-3.39670	2.33341	-0.09301
C	-3.01262	1.00031	0.11573
C	-3.99146	0.02520	0.35294
C	-5.35092	0.38223	0.35255
H	-5.04636	3.72328	-0.26875
H	-2.64335	3.10803	-0.27960
H	-3.70931	-1.02070	0.52473
H	-6.10868	-0.39247	0.53008
I	-1.26494	0.21341	-2.51675
C	-7.22151	2.08646	0.08866
H	-7.59168	2.13786	-0.95381
H	-7.84582	1.35029	0.62381
H	-7.39778	3.07865	0.54153

E(DMF)= -1845.944353122972; G= 0.33797037

Pd(PPh₃)(CO)(PhIF) (11e)

Pd	-1.00691	0.45114	0.09934
P	1.35007	-0.14586	0.04157
C	1.91535	-1.57021	-0.97210
C	2.17617	-2.82847	-0.39451
C	2.03092	-1.41045	-2.37030
C	2.54914	-3.91130	-1.20435
H	2.09844	-2.96592	0.68898
C	2.40803	-2.49611	-3.17153
H	1.82777	-0.43849	-2.82872
C	2.66497	-3.74880	-2.59294
H	2.75562	-4.88485	-0.74408
H	2.49702	-2.35988	-4.25586
H	2.95774	-4.59675	-3.22318
C	1.98070	-0.53491	1.73069
C	3.19634	-0.02883	2.22816
C	1.19553	-1.37467	2.54901
C	3.62097	-0.36379	3.52301
H	3.80958	0.63340	1.60832
C	1.62832	-1.71553	3.83725
H	0.23967	-1.75954	2.17465
C	2.84229	-1.20886	4.32752
H	4.56614	0.03996	3.90345
H	1.01046	-2.36974	4.46361
H	3.17599	-1.46743	5.33870
C	2.37021	1.26283	-0.53876
C	3.69578	1.08169	-0.98457
C	1.81761	2.55789	-0.50937
C	4.45870	2.18687	-1.38553
H	4.12565	0.07458	-1.02514
C	2.58546	3.66090	-0.90930
H	0.77809	2.69425	-0.18823
C	3.90582	3.47724	-1.34661
H	5.48716	2.03906	-1.73436
H	2.14584	4.66506	-0.88933
H	4.50281	4.33918	-1.66637
C	-1.09138	0.84116	1.94957
O	-1.19554	1.14224	3.05534
C	-5.71110	1.70482	0.11115
C	-4.74605	2.69550	-0.09776
C	-3.38802	2.33415	-0.09229
C	-3.00995	0.99734	0.11015
C	-3.99368	0.02039	0.33089
C	-5.35525	0.36932	0.32706
H	-5.06227	3.73022	-0.26953
H	-2.63113	3.10668	-0.27130
H	-3.71447	-1.02791	0.49062
H	-6.13823	-0.38032	0.48571
I	-1.26341	0.19720	-2.51532
F	-7.01811	2.04584	0.10627

E(DMF)= -1905.901926929404; G= 0.30358685

Pd(PPh₃)(CO)(PhICl) (11f)

Pd	-1.00455	0.45398	0.09943
P	1.35176	-0.14391	0.04182
C	1.91448	-1.56825	-0.97292
C	2.17580	-2.82653	-0.39556
C	2.02647	-1.40895	-2.37145
C	2.54630	-3.90973	-1.20601
H	2.10053	-2.96361	0.68812
C	2.40124	-2.49499	-3.17327
H	1.82253	-0.43710	-2.82973

C	2.65897	-3.74760	-2.59490
H	2.75334	-4.88328	-0.74602
H	2.48762	-2.35917	-4.25785
H	2.94975	-4.59587	-3.22561
C	1.98123	-0.53359	1.73107
C	3.19697	-0.02808	2.22885
C	1.19549	-1.37326	2.54894
C	3.62104	-0.36333	3.52380
H	3.81071	0.63391	1.60920
C	1.62776	-1.71439	3.83729
H	0.23966	-1.75788	2.17425
C	2.84173	-1.20816	4.32797
H	4.56626	0.03997	3.90456
H	1.00952	-2.36848	4.46339
H	3.17505	-1.46699	5.33920
C	2.37216	1.26454	-0.53810
C	3.69940	1.08368	-0.97909
C	1.81851	2.55926	-0.51259
C	4.46269	2.18876	-1.37956
H	4.13038	0.07693	-1.01605
C	2.58672	3.66216	-0.91211
H	0.77796	2.69554	-0.19478
C	3.90861	3.47874	-1.34488
H	5.49247	2.04120	-1.72454
H	2.14630	4.66602	-0.89526
H	4.50596	4.34058	-1.66419
C	-1.08138	0.85753	1.94772
O	-1.18127	1.16646	3.05158
C	-5.72069	1.69734	0.11392
C	-4.74980	2.68677	-0.09934
C	-3.39148	2.32864	-0.09728
C	-3.00803	0.99387	0.10601
C	-3.98976	0.01608	0.32987
C	-5.35161	0.36150	0.32985
H	-5.05570	3.72397	-0.27184
H	-2.63825	3.10426	-0.27912
H	-3.70946	-1.03192	0.49035
H	-6.12256	-0.39859	0.49392
I	-1.26470	0.18424	-2.51268
Cl	-7.41871	2.13617	0.11275

E(DMF)= -2266.249306769136; G= 0.30321660

Pd(PPh₃)(CO)(PhICF₃) (11g)

Pd	-1.00379	0.45817	0.09411
P	1.35150	-0.14223	0.04028
C	1.91188	-1.56689	-0.97427
C	2.16525	-2.82692	-0.39713
C	2.03013	-1.40629	-2.37211
C	2.53428	-3.91070	-1.20739
H	2.08498	-2.96483	0.68608
C	2.40359	-2.49298	-3.17366
H	1.83288	-0.43291	-2.83011
C	2.65339	-3.74732	-2.59561
H	2.73523	-4.88569	-0.74780
H	2.49523	-2.35633	-4.25767
H	2.94311	-4.59607	-3.22611
C	1.97464	-0.53309	1.73121
C	3.19028	-0.03017	2.23176
C	1.18466	-1.37065	2.54719
C	3.61004	-0.36572	3.52802
H	3.80719	0.63008	1.61339
C	1.61268	-1.71201	3.83689
H	0.22893	-1.75333	2.17022
C	2.82653	-1.20829	4.33050
H	4.55512	0.03561	3.91115
H	0.99130	-2.36433	4.46169
H	3.15650	-1.46731	5.34276
C	2.37284	1.26593	-0.53737
C	3.70175	1.08463	-0.97328

C	1.81899	2.56065	-0.51521
C	4.46629	2.18937	-1.37224
H	4.13315	0.07796	-1.00755
C	2.58850	3.66316	-0.91331
H	0.77745	2.69757	-0.20097
C	3.91193	3.47932	-1.34110
H	5.49732	2.04152	-1.71329
H	2.14799	4.66700	-0.89911
H	4.51035	4.34085	-1.65918
C	-1.06658	0.87964	1.94011
O	-1.15781	1.19926	3.04137
C	-5.72615	1.71209	0.09773
C	-4.74248	2.69129	-0.11001
C	-3.38424	2.33532	-0.11034
C	-3.00471	0.99934	0.08828
C	-3.98906	0.01998	0.30548
C	-5.34521	0.37367	0.30554
H	-5.03552	3.73249	-0.27923
H	-2.62832	3.10878	-0.28880
H	-3.70842	-1.02878	0.45818
H	-6.11082	-0.39423	0.46371
I	-1.26946	0.15860	-2.51314
C	-7.19211	2.07011	0.13921
F	-7.42892	3.34445	-0.24886
F	-7.93047	1.26072	-0.66170
F	-7.70106	1.93589	1.39376

E(DMF)= -2143.728983147011; G= 0.31573028

Pd(PPh₃)(CO)(PhICN) (11h)

Pd	-1.00278	0.46184	0.10579
P	1.35112	-0.13839	0.04551
C	1.90381	-1.56211	-0.97385
C	2.15045	-2.82519	-0.40049
C	2.02278	-1.39768	-2.37118
C	2.51371	-3.90831	-1.21415
H	2.06971	-2.96590	0.68231
C	2.39063	-2.48376	-3.17609
H	1.83118	-0.42181	-2.82626
C	2.63366	-3.74118	-2.60186
H	2.70955	-4.88577	-0.75767
H	2.48317	-2.34426	-4.25963
H	2.91880	-4.58947	-3.23500
C	1.97575	-0.53392	1.73441
C	3.19240	-0.03256	2.23412
C	1.18644	-1.37288	2.54965
C	3.61385	-0.37114	3.52904
H	3.80865	0.62884	1.61641
C	1.61620	-1.71709	3.83800
H	0.22995	-1.75444	2.17340
C	2.83104	-1.21500	4.33082
H	4.55962	0.02892	3.91167
H	0.99556	-2.37054	4.46232
H	3.16236	-1.47638	5.34200
C	2.37227	1.26915	-0.53264
C	3.69969	1.08573	-0.97239
C	1.82074	2.56483	-0.50790
C	4.46508	2.18947	-1.37231
H	4.12914	0.07832	-1.00888
C	2.59114	3.66632	-0.90711
H	0.78043	2.70355	-0.19044
C	3.91308	3.48038	-1.33854
H	5.49490	2.04011	-1.71624
H	2.15261	4.67098	-0.89082
H	4.51217	4.34108	-1.65750
C	-1.04794	0.89244	1.95125
O	-1.12889	1.21754	3.05148
C	-5.73527	1.69396	0.10628
C	-4.74691	2.67988	-0.11823
C	-3.39168	2.32780	-0.11622

C	-3.00463	0.99381	0.09924
C	-3.98397	0.01271	0.33246
C	-5.34200	0.35453	0.33228
H	-5.05017	3.71701	-0.29895
H	-2.63828	3.10106	-0.30544
H	-3.69678	-1.03195	0.50003
H	-6.10666	-0.41075	0.50462
I	-1.28061	0.14818	-2.49727
C	-7.12513	2.04984	0.10942
N	-8.26025	2.33980	0.11349

E(DMF)= -1898.873921645703; G= 0.31078487

Pd(PPh₃)(CO)(PhINO₂) (11i)

Pd	-0.99966	0.45890	0.10953
P	1.35445	-0.13914	0.04697
C	1.90661	-1.56210	-0.97353
C	2.15234	-2.82575	-0.40108
C	2.02605	-1.39649	-2.37067
C	2.51517	-3.90837	-1.21558
H	2.07124	-2.96735	0.68157
C	2.39351	-2.48208	-3.17640
H	1.83531	-0.42007	-2.82495
C	2.63558	-3.74012	-2.60312
H	2.71028	-4.88632	-0.75989
H	2.48649	-2.34173	-4.25979
H	2.92040	-4.58804	-3.23689
C	1.98037	-0.53462	1.73523
C	3.19743	-0.03314	2.23376
C	1.19192	-1.37392	2.55096
C	3.62017	-0.37199	3.52818
H	3.81291	0.62862	1.61564
C	1.62300	-1.71835	3.83881
H	0.23517	-1.75570	2.17556
C	2.83826	-1.21616	4.33051
H	4.56623	0.02816	3.91000
H	1.00310	-2.37206	4.46359
H	3.17061	-1.47771	5.34130
C	2.37260	1.27001	-0.53203
C	3.70049	1.08874	-0.97130
C	1.81854	2.56463	-0.50839
C	4.46377	2.19365	-1.37199
H	4.13196	0.08217	-1.00685
C	2.58684	3.66727	-0.90844
H	0.77795	2.70177	-0.19119
C	3.90922	3.48351	-1.33946
H	5.49396	2.04603	-1.71554
H	2.14632	4.67106	-0.89308
H	4.50668	4.34511	-1.65900
C	-1.04018	0.89499	1.95394
O	-1.11859	1.22328	3.05329
C	-5.70151	1.68409	0.10589
C	-4.74115	2.67933	-0.12054
C	-3.38557	2.32547	-0.11774
C	-3.00040	0.98979	0.09952
C	-3.98020	0.00755	0.33404
C	-5.33904	0.34961	0.33416
H	-5.06887	3.70701	-0.29880
H	-2.63097	3.09735	-0.30701
H	-3.69253	-1.03669	0.50244
H	-6.12120	-0.39461	0.50595
I	-1.28220	0.13589	-2.49154
N	-7.13764	2.05303	0.10745
O	-7.95412	1.16020	0.31733
O	-7.42348	3.22904	-0.09939

E(DMF)= -2011.147678343041; G= 0.31355234

trans-Pd(PPh₃)₂(Ph)(I)

Pd	-0.72636	-0.32597	0.09302
P	-2.89543	0.26695	0.73266
P	1.32566	-1.10435	-0.70571
H	-5.43608	4.02776	-2.79292
H	2.49999	1.31686	-5.78147
H	0.17056	0.59948	-5.20424
H	0.79812	-5.15768	-3.59414
H	-3.60279	2.53556	-3.62308
C	2.29249	0.85361	-4.80985
C	0.98667	0.44968	-4.48761
C	-4.94645	3.32435	-2.10874
C	-3.92288	2.48550	-2.57577
C	1.00114	-4.78350	-2.58345
H	1.01005	-2.70941	-3.20769
H	1.02866	-6.75906	-1.68425
H	4.34415	1.00922	-4.11976
C	3.32697	0.67825	-3.87946
C	0.71978	-0.12254	-3.23827
H	-0.30405	-0.40338	-2.96436
C	1.12126	-3.40204	-2.36728
H	-6.12733	3.93023	-0.38900
C	1.13499	-5.68058	-1.51476
C	-5.33448	3.26987	-0.76105
C	-3.28863	1.59663	-1.69792
H	-2.46521	0.96543	-2.04818
C	3.06650	0.08890	-2.63267
C	1.76156	-0.31839	-2.30858
I	0.04848	2.29199	-0.29874
C	1.37849	-2.90890	-1.07505
C	1.40309	-5.19233	-0.22564
C	-4.70920	2.37372	0.11798
H	3.87658	-0.03335	-1.90652
C	-3.68560	1.52939	-0.34825
H	-0.94172	1.54661	2.46251
H	1.50142	-5.88464	0.61798
C	1.52679	-3.81676	-0.00624
H	-5.01390	2.34151	1.16916
H	4.02179	-2.32532	-0.59287
H	-1.97018	-2.84211	-1.31502
H	-1.04012	2.44879	4.79041
C	-1.87135	1.48552	3.04024
H	1.71874	-3.44386	1.00430
H	-4.83762	-0.63640	-1.30595
C	3.95307	-1.59666	0.22267
C	-1.93406	1.99773	4.34392
C	2.76138	-0.86556	0.41294
C	-1.74960	-3.14721	-0.28608
H	-2.47909	-5.16234	-0.59812
C	-3.01325	0.90683	2.45180
C	-2.03863	-4.45860	0.11848
H	5.96773	-1.97059	0.92526
C	-1.18018	-2.23080	0.61518
C	5.04397	-1.40032	1.08010
C	-4.86795	-1.35321	-0.47784
C	-4.10637	-1.11978	0.68289
C	2.67294	0.05522	1.47407
H	1.75164	0.63236	1.61037
C	-3.13199	1.93417	5.07200
H	-6.24902	-2.67787	-1.49175
H	-3.17736	2.33187	6.09246
C	-5.66132	-2.50560	-0.58189
C	-1.76322	-4.87111	1.43212
C	-0.90451	-2.64785	1.93088
C	4.95266	-0.47851	2.13561
C	-4.21583	0.84434	3.18731
C	3.76721	0.24583	2.33097
H	-1.98958	-5.89669	1.74722
H	-0.46091	-1.94636	2.64914
C	-4.27229	1.35652	4.49119
C	-1.19614	-3.96250	2.33746
C	-4.15674	-2.05087	1.73981
H	5.80675	-0.32751	2.80714

H	-5.10499	0.38298	2.74449
H	-3.55328	-1.89246	2.63769
H	3.69060	0.96674	3.15372
C	-5.70184	-3.43226	0.46972
H	-0.97621	-4.27432	3.36655
C	-4.94978	-3.19822	1.63193

H	-5.21061	1.30074	5.05635
H	-6.31572	-4.33703	0.38415
H	-4.96568	-3.92187	2.45547

E(DMF)= -2729.348812650870; G= 0.57090828