

Electronic Supplementary Information (ESI)

New Palladium(II) and Platinum(II) Complexes with the Model Nucleobase 9-Methylhypoxanthine: Crystal Structures and Theoretical Calculations.

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Table SI 1. Selected geometrical parameters (distances in Å and angles in degrees) for the experimental (X-ray diffraction) and calculated (method A and B) structures of complexes **2** and **6**.

	2			6		
	Exp.	Calc.A	Calc.B	Exp.	Calc.A	Calc.B
Pt1-P1	2.2333(5)	2.285	2.263	2.2148(9)	2.265	2.244
Pt1-C1	2.016(2)	2.028	2.027	2.017(3)	2.043	2.041
Pt1-N1	2.1390(17)	2.196	2.197	2.138(3)	2.196	2.197
Pt1-N2	2.1253(18)	2.172	2.158	2.108(3)	2.156	2.147
C1-Pt1-P1	94.34(6)	95.51	95.18	94.94(11)	96.43	95.94
P1-Pt1-N2	91.64(5)	91.62	92.45	93.18(8)	92.40	93.18
N1-Pt1-N2	92.67(7)	92.55	92.04	90.25(11)	90.68	90.42
Pt1-N2-C15	131.05(14)	126.22	126.79	-	-	-
Pt1-N2-C14	-	-	-	117.8(2)	116.76	116.41

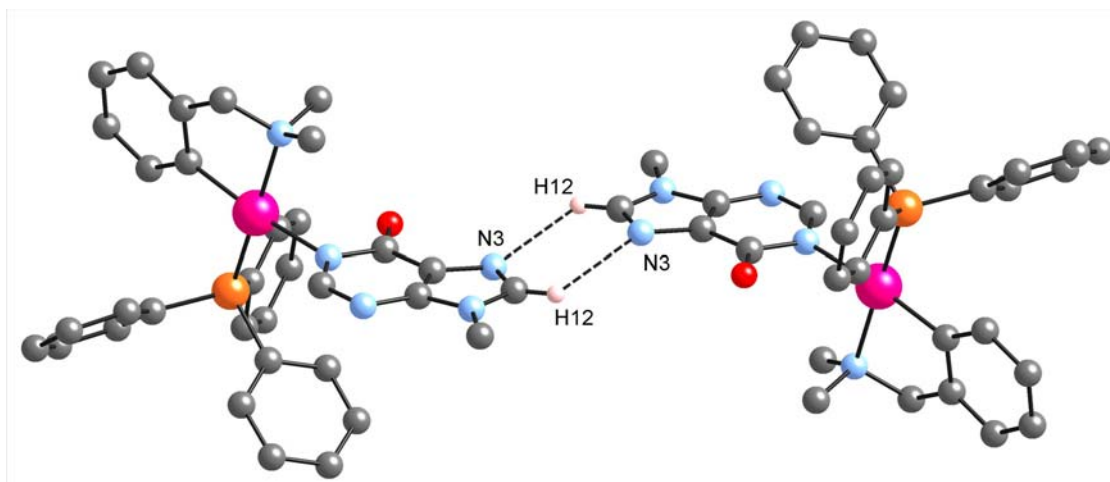


Figure SI 1. Association of molecules of **6** via C(12)H12...N(3) bonds

Calculated structures.- Cartesian coordinates (Å) and energies (au) for all calculated species.-

Compound 9-mhpyH (method B): E = -526.718992739 au

N	0.00000000	0.00000000	0.00000000	H	-0.50001912	-0.88901911	-0.00000000
C	1.36530617	0.00000000	0.00000000	H	1.84769011	-0.98112201	0.00000000
N	2.10416382	1.08134353	0.00000000	O	-2.07843892	1.01073722	-0.00000000
C	1.35262645	2.21675676	0.00000000	H	0.84273157	5.41417910	0.00000000
C	-0.04583896	2.34912902	0.00000000	C	3.25299257	3.88184725	-0.00000000
C	-0.86495432	1.15689348	0.00000000	H	3.49557482	4.46901650	-0.89672358
N	-0.40883274	3.67806800	0.00000000	H	3.84739578	2.96043634	-0.00000000
C	0.73782249	4.33097968	0.00000000	H	3.49557934	4.46900330	0.89673143
N	1.84613659	3.50353550	-0.00000000				

Compound 9-mhpyH·ClO₄⁻ (method B): E = -1287.87960393 au

N	0.00000000	0.00000000	0.00000000	O	-2.06912307	1.05208590	0.00743776
C	1.35879911	0.00000000	0.00000000	H	0.87604362	5.42101249	0.00069831
N	2.11666774	1.08222663	0.00000000	C	3.27770000	3.86140199	-0.00349393
C	1.36972031	2.21460810	0.00000000	H	3.53541509	4.44270863	-0.90165053
C	-0.02499088	2.35172101	0.00187731	H	3.85259186	2.92638478	-0.00304696
C	-0.84682129	1.15482149	0.00314971	H	3.53841217	4.44566354	0.89188162
N	-0.38284024	3.68849155	0.00280001	O	-0.75116807	-2.73763766	0.06736527
C	0.76522121	4.33782927	0.00107745	Cl	0.30094876	-3.74201852	-0.27129564
N	1.87017403	3.50432470	-0.00052430	O	1.61085218	-3.22336836	0.17942390
H	-0.44913681	-0.94359057	-0.00180943	O	0.32221399	-3.94713583	-1.72286384
H	1.81424379	-0.99581644	0.00184594	O	-0.00423966	-4.99437858	0.42204554

Compound 9-mhpy⁻ (method B): E = -526.164346263 au

N	0.00000000	0.00000000	0.00000000	N	2.09362722	3.46972999	0.00000000
C	1.32844595	0.00000000	0.00000000	H	1.80246475	-0.99505398	-0.00000000
N	2.21082080	1.03223563	0.00000000	O	-1.96513547	1.23284938	0.00000000
C	1.53167126	2.19587034	0.00000000	H	1.18837756	5.43262423	0.00000000
C	0.14243719	2.39300748	0.00000000	C	3.51134267	3.75256549	0.00000000
C	-0.72052687	1.21340941	0.00000000	H	3.81276402	4.32077046	-0.89611285
N	-0.14918649	3.75545619	0.00000000	H	4.03081461	2.78359388	0.00000000
C	1.02544624	4.35471924	0.00000000	H	3.81277255	4.32073645	0.89613214

Complex [Pt(PPh₃)(dmap)]⁺ (method B): E = -1561.00409996 au

Pt	0.00000000	0.00000000	0.00000000	H	1.86167961	-3.35331384	-0.63850660
C	1.99406428	0.00000000	0.00000000	N	0.17815178	-2.02282134	-0.75303299
C	2.90106032	1.06144237	0.00000000	C	0.31697086	-2.01754007	-2.23788223
C	4.27682821	0.79778460	-0.06362861	H	0.47248834	-3.04752320	-2.60269035
C	4.75216652	-0.51062994	-0.14801589	H	1.17373401	-1.39650891	-2.52289917
C	3.84558994	-1.57266964	-0.18113283	H	-0.59379168	-1.60720628	-2.69075321
C	2.46889349	-1.33133884	-0.10982130	C	-0.93299114	-2.92778586	-0.35955228
H	2.58134626	2.10006806	0.04877036	H	-1.86456446	-2.58298444	-0.82769413
H	4.97392296	1.63767745	-0.05372942	H	-1.04840082	-2.91694031	0.73127486
H	5.82427214	-0.70410393	-0.20294203	H	-0.73074748	-3.95992070	-0.69421960
H	4.20731286	-2.60049963	-0.26773414	P	-0.00000065	2.12291927	0.79036503
C	1.47065378	-2.46347954	-0.11487225	C	0.23271841	3.44386596	-0.45391746
H	1.22509468	-2.76293911	0.91619960	C	0.77304048	3.15892732	-1.71900502

C	0.90795335	4.17415636	-2.67003998	H	3.04079174	4.83400312	3.67817021
C	0.50275465	5.47690859	-2.36809139	H	3.18892959	3.07801811	5.44026419
C	-0.05017381	5.76480895	-1.11533643	H	1.98077468	0.91674714	5.14552451
C	-0.19164594	4.75488568	-0.16235105	H	0.64032199	0.50957998	3.09534032
H	1.07818989	2.13985872	-1.96199363	C	-1.73181688	2.35321107	1.35848343
H	1.32576996	3.94333056	-3.65142554	C	-2.74828775	2.19787063	0.39293001
H	0.60699912	6.26795533	-3.11269500	C	-4.09058636	2.29385601	0.76316924
H	-0.38204762	6.77784607	-0.88167265	C	-4.43218551	2.54535239	2.09660355
H	-0.65204090	4.98385743	0.80085832	C	-3.42845597	2.70180515	3.05698545
C	1.05702382	2.45816644	2.24011001	C	-2.08155153	2.60269216	2.69460536
C	1.74240728	3.67211724	2.40720251	H	-2.48685741	2.03060595	-0.65590826
C	2.50743981	3.88964065	3.55697825	H	-4.87092367	2.18062933	0.00855054
C	2.59030414	2.90442133	4.54443874	H	-5.48156534	2.62480526	2.38539870
C	1.91189993	1.69171446	4.38024548	H	-3.69279182	2.90618765	4.09602238
C	1.15350670	1.46435475	3.23106507	H	-1.30598768	2.72611413	3.45176425
H	1.69083651	4.44630471	1.64032121				

Complex [Pt(PPh₃)(dmap)(N7-9mhypH)] (method A): E = -2087.18376645 au

Pt	0.00000000	0.00000000	0.00000000	C	2.33173347	3.80580138	3.75765823
C	2.02894396	0.00000000	0.00000000	C	2.65947526	2.70680526	4.56778002
C	2.92216041	1.09261315	0.00000000	C	2.15400250	1.43335313	4.25847108
C	4.31383394	0.89906214	-0.07035691	C	1.32289335	1.25940375	3.14165643
C	4.85057505	-0.39420388	-0.14697978	H	1.25208924	4.50363587	2.01756581
C	3.98399194	-1.49754474	-0.17308585	H	2.73528539	4.79722738	3.98630224
C	2.59415550	-1.30450215	-0.10004124	H	3.31735680	2.84044102	5.43220498
H	2.54826323	2.11931544	0.05078110	H	2.42050494	0.57017215	4.87652353
H	4.97802573	1.76981341	-0.06690700	H	0.96253189	0.26106849	2.86900574
H	5.93315856	-0.54372916	-0.20275577	C	-1.85562778	2.41675571	1.69695466
H	4.38905183	-2.51295891	-0.25686040	C	-2.93276995	2.82370271	0.87703845
C	1.62447894	-2.45579993	-0.14507862	C	-4.20342119	3.04331928	1.43225353
H	1.31859984	-2.76829420	0.87040711	C	-4.41586978	2.85520240	2.81005471
H	2.03485353	-3.34482192	-0.66452378	C	-3.35060654	2.44748690	3.62981555
N	0.36912977	-1.99653705	-0.84887560	C	-2.07575418	2.22966066	3.07843095
C	0.62665127	-1.86634266	-2.32004799	H	-2.77275936	2.98924774	-0.19333255
H	0.81113394	-2.86770635	-2.75538937	H	-5.02451080	3.37956029	0.79063585
H	1.51010699	-1.23163782	-2.47285793	H	-5.40230916	3.04676058	3.24475311
H	-0.23996281	-1.39075898	-2.80124086	H	-3.50280270	2.31756372	4.70621301
C	-0.71519976	-2.99088942	-0.63053440	H	-1.24658280	1.93527638	3.72965975
H	-1.61680815	-2.68059924	-1.17759169	N	-4.08832861	0.26144974	-3.21434459
H	-0.94330398	-3.05934371	0.44376894	C	-5.32554163	0.03314618	-2.66377779
H	-0.39720967	-3.98487324	-0.99958183	N	-5.53087470	-0.26853768	-1.39810902
P	-0.19556090	2.07988566	0.93758800	C	-4.37288602	-0.32587937	-0.68286200
C	-0.00891930	3.44619032	-0.28271415	C	-3.05935452	-0.10827819	-1.13322192
C	0.48780325	3.15591324	-1.57199933	C	-2.82667516	0.20309939	-2.52798292
C	0.64396430	4.18446401	-2.51498210	N	-2.17715273	-0.26513279	-0.07363244
C	0.30425910	5.50487487	-2.18178902	C	-2.94068610	-0.56920344	0.98150939
C	-0.20814541	5.79829763	-0.90618716	N	-4.27422155	-0.62356742	0.66532922
C	-0.37173991	4.77551606	0.03993234	H	-4.01628626	0.48160029	-4.21183675
H	0.73365951	2.12143713	-1.83359306	H	-6.17982763	0.11179650	-3.34378612
H	1.02666469	3.94859846	-3.51274810	O	-1.76932758	0.39483771	-3.13543222
H	0.42794766	6.30547571	-2.91792753	H	-2.56772604	-0.73373464	1.99012370
H	-0.48760818	6.82461860	-0.64786996	C	-5.39497068	-0.89189063	1.57446953
H	-0.80044060	5.01065783	1.01964071	H	-5.21770819	-1.82980981	2.12138437
C	0.97592056	2.36513903	2.33396518	H	-6.30334100	-0.98719247	0.96408378
C	1.48947229	3.64084430	2.64627846	H	-5.51068338	-0.05676232	2.28207127

Complex [Pt(PPh₃)(dmap)(N3-9mhypH·ClO₄)] (method A): E = -2848.17786261 au

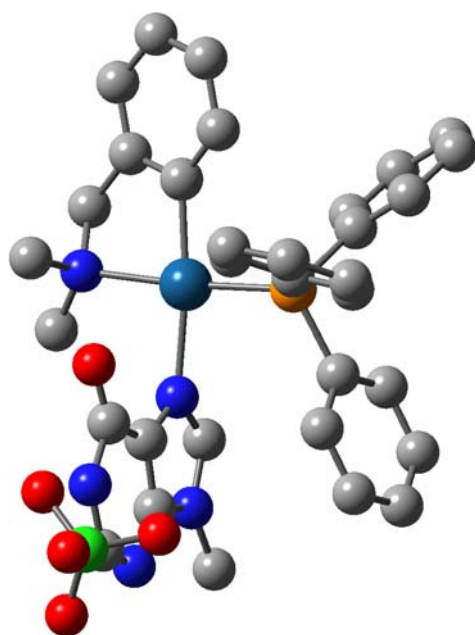
Pt	0.00000000	0.00000000	0.00000000	C	4.32428953	0.87618022	-0.02878206
C	2.02880295	0.00000000	0.00000000	C	4.84895976	-0.42383145	-0.05814124
C	2.93280757	1.08374029	0.00000000	C	3.97157891	-1.51960163	-0.06947855

C	2.58235828	-1.31304616	-0.03764344	H	3.31230535	2.59026319	5.52921048
H	2.56681066	2.11414199	0.03285393	H	2.24121077	0.38379971	4.99724246
H	4.99736990	1.74061582	-0.02329538	H	0.76555593	0.15300232	3.02376466
H	5.93143977	-0.58568638	-0.07891227	C	-1.89404752	2.28050306	1.77786262
H	4.36774453	-2.54162484	-0.10089527	C	-2.96720673	2.72557178	0.97263505
C	1.60197521	-2.45696560	-0.03653030	C	-4.25799807	2.83527323	1.51043604
H	1.26570476	-2.70471325	0.98662540	C	-4.49400389	2.49296864	2.85350225
H	2.01558799	-3.37853157	-0.49386516	C	-3.43386454	2.04359114	3.65543444
N	0.36525099	-2.03307330	-0.79550381	C	-2.13723890	1.93575449	3.12406235
C	0.66147969	-1.96539665	-2.25773837	H	-2.79403000	2.99409006	-0.07480601
H	0.93947664	-2.97075738	-2.63099292	H	-5.08088112	3.18433069	0.87836511
H	1.49037868	-1.26580941	-2.43433057	H	-5.50322580	2.57159255	3.26972524
H	-0.23568733	-1.62114840	-2.79353292	H	-3.60940343	1.76462959	4.69882392
C	-0.71349151	-3.03837036	-0.56454241	H	-1.32541219	1.57105870	3.75946375
H	-1.61962650	-2.74237288	-1.11333801	N	-3.79831580	-1.51877096	1.35181458
H	-0.92528150	-3.12102126	0.51310982	C	-2.57961134	-0.96438245	1.18340897
H	-0.37781928	-4.02509515	-0.93810006	N	-2.17505091	-0.36949867	0.05837806
P	-0.22135335	2.03121256	1.02701770	C	-3.14071859	-0.33846731	-0.92300116
C	-0.02502321	3.49387763	-0.08486372	C	-4.43699552	-0.88361191	-0.83169552
C	0.58307253	3.33902612	-1.34912033	C	-4.86921616	-1.55680654	0.38435903
C	0.75451426	4.44660569	-2.19534150	N	-5.13913120	-0.67047139	-2.00275616
C	0.31748958	5.71759392	-1.78970038	C	-4.29341024	-0.01262120	-2.77820968
C	-0.29627366	5.87978870	-0.53619456	N	-3.05550956	0.22014294	-2.18656309
C	-0.47023429	4.77589288	0.31296083	H	-3.91994357	-2.01682440	-2.25243906
H	0.91871143	2.34411981	-1.66119439	H	-1.88797207	-1.02110165	2.03482143
H	1.23058405	4.31424546	-3.17244888	O	-5.94039149	-2.09705291	0.65035546
H	0.44997938	6.58053032	-2.45032741	H	-4.50098407	0.33007466	-3.79256995
H	-0.64533864	6.86748395	-0.21804648	C	-1.95319741	0.98917852	-2.76250686
H	-0.96744433	4.90773652	1.27932047	H	-1.77978404	0.66929620	-3.80215475
C	0.95290381	2.24892998	2.43085877	H	-1.04426697	0.80304819	-2.15845532
C	1.55017376	3.49042336	2.73200724	H	-2.17427241	2.06919142	-2.74292238
C	2.40088149	3.60702736	3.84291867	Cl	-1.34563533	-2.80916477	3.88286477
C	2.65085213	2.49417406	4.66199129	O	-2.87497090	-2.78085158	3.80002448
C	2.05547345	1.25740010	4.36507318	O	-0.83868095	-1.36025145	3.79079022
C	1.21670832	1.12648198	3.24775835	O	-0.90529687	-3.43571197	5.17019114
H	1.36560119	4.36334055	2.09877782	O	-0.79785189	-3.57898042	2.68470263
H	2.86879335	4.57164377	4.06562674				

Complex [Pt(PPh₃)(dmap)(N7-9mhyphH·ClO₄)] (method A): E = -2848.1818247 au

Pt	0.00000000	0.00000000	0.00000000	C	0.33034248	3.10563290	-1.63432295
C	2.02846318	0.00000000	0.00000000	C	0.40210794	4.10942090	-2.61360926
C	2.92463632	1.09120375	0.00000000	C	0.09527007	5.43827114	-2.28558467
C	4.31582016	0.89857648	-0.07952923	C	-0.29940072	5.76686449	-0.97686703
C	4.85258406	-0.39426887	-0.16852767	C	-0.38569039	4.76908059	0.00435287
C	3.98473695	-1.49684175	-0.20193905	H	0.52638318	2.06148167	-1.89850431
C	2.59558519	-1.30317645	-0.11963683	H	0.67089194	3.84161277	-3.63952278
H	2.54767258	2.11724655	0.05155757	H	0.13659535	6.21560199	-3.05489962
H	4.98033073	1.76956139	-0.07674007	H	-0.56347819	6.79883003	-0.72456234
H	5.93516544	-0.54353167	-0.23258841	H	-0.74562152	5.02737323	1.00579610
H	4.38855307	-2.51178508	-0.30199010	C	0.95494054	2.38705404	2.31532315
C	1.62196906	-2.45204461	-0.18568005	C	1.48702450	3.66081789	2.60140903
H	1.31445148	-2.78102838	0.82441308	C	2.33457330	3.83806442	3.70702681
H	2.03182295	-3.33302506	-0.72059958	C	2.65054442	2.75236347	4.53915691
N	0.36944383	-1.97816577	-0.88029757	C	2.12861218	1.47970547	4.25555129
C	0.62251099	-1.81342293	-2.34908469	C	1.29270431	1.29446431	3.14404574
H	0.78410036	-2.80740814	-2.81076441	H	1.25908646	4.51218642	1.95403742
H	1.51793119	-1.19251981	-2.48858949	H	2.75133591	4.82915987	3.91383758
H	-0.23367775	-1.30003546	-2.81111864	H	3.31223740	2.89514865	5.39962013
C	-0.72292084	-2.96686744	-0.68416564	H	2.38620015	0.62491861	4.88937633
H	-1.62148698	-2.63046980	-1.21996157	H	0.92033832	0.29578524	2.88874977
H	-0.95072081	-3.05787701	0.38861924	C	-1.87831589	2.41605295	1.68318852
H	-0.41438088	-3.95433049	-1.07964966	C	-2.94363307	2.85554843	0.86486359
P	-0.21953585	2.07914878	0.92094204	C	-4.21601819	3.07527603	1.41659337
C	-0.05508675	3.43013820	-0.31589800	C	-4.43932056	2.85837588	2.78773187

C	-3.38447605	2.42066840	3.60607638	N	-4.30593748	-0.50920948	0.47618969
C	-2.10923225	2.19954355	3.05862421	H	-3.70662629	1.31219430	-4.21707842
H	-2.78045619	3.04174994	-0.20111871	H	-5.85755437	0.99728357	-3.48757814
H	-5.02759238	3.42718924	0.77178520	O	-1.48488363	0.63606918	-3.03316868
H	-5.42817980	3.04682279	3.21881832	H	-2.69149480	-0.86486095	1.87499237
H	-3.54643224	2.26587863	4.67811052	C	-5.49828784	-0.76340906	1.28647013
H	-1.28867461	1.87787404	3.70805731	H	-5.48118468	-1.79065152	1.68262665
N	-3.80065680	0.82469017	-3.26150208	H	-6.37000917	-0.63721620	0.62870024
C	-5.07344050	0.66914806	-2.79436918	H	-5.55566019	-0.03986075	2.11464911
N	-5.40372391	0.19738650	-1.59370126	Cl	-4.91314244	3.29974174	-5.38751898
C	-4.30671254	-0.06625205	-0.84237999	O	-3.84819420	2.17464782	-5.58464442
C	-2.96003566	0.08083057	-1.20148227	O	-6.23571796	2.62583193	-5.04750803
C	-2.61890652	0.52331489	-2.53883219	O	-4.47087717	4.17171228	-4.23138134
N	-2.15465935	-0.24340423	-0.11661660	O	-5.01884541	4.08271040	-6.66208034
C	-2.99276625	-0.58657083	0.86758200				



Complex [Pt(PPh₃)(dmap)(N7-9mhyph·ClO₄)] (method B): E = -2848.1818247 au

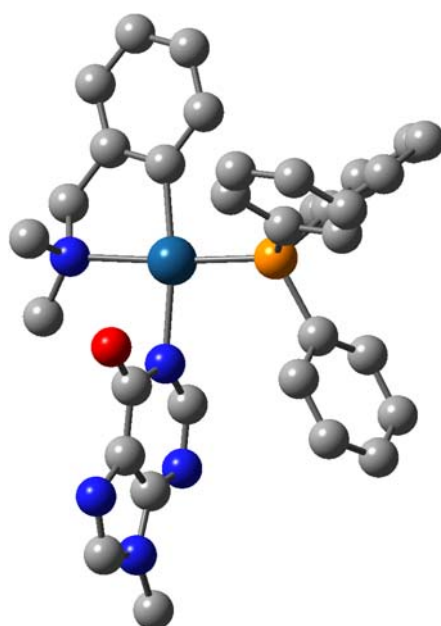
Pt	0.00000000	0.00000000	0.00000000	C	-0.00611867	3.40798421	-0.38134719
C	2.02749959	0.00000000	0.00000000	C	0.40896913	3.07279665	-1.68042901
C	2.92639691	1.08079358	0.00000000	C	0.51955589	4.06279562	-2.66093039
C	4.31113937	0.88405298	-0.06361904	C	0.22065296	5.39155585	-2.35372683
C	4.84165381	-0.40574894	-0.13664141	C	-0.20579810	5.73232560	-1.06487479
C	3.97180124	-1.49884652	-0.16619282	C	-0.32856209	4.74742137	-0.08417259
C	2.58855639	-1.29993984	-0.09921373	H	0.60423284	2.02884017	-1.93022837
H	2.55804150	2.10675112	0.04459813	H	0.81585816	3.78504242	-3.67344639
H	4.97698908	1.75003595	-0.06221776	H	0.29417930	6.16070479	-3.12469619
H	5.92098737	-0.55965010	-0.18895506	H	-0.46476119	6.76602483	-0.82813233
H	4.37131970	-2.51350103	-0.25175313	H	-0.70924730	5.01800798	0.90256287
C	1.62131369	-2.44715844	-0.15275393	C	0.95096038	2.40901329	2.26226027
H	1.32324194	-2.76734564	0.85934013	C	1.51782444	3.66928024	2.50727487
H	2.03637893	-3.32796904	-0.67684422	C	2.35488203	3.86311027	3.61007756
N	0.36870704	-1.99367392	-0.84689037	C	2.62759599	2.80652409	4.48317496
C	0.62074256	-1.85328886	-2.31329072	C	2.07181011	1.54642431	4.24198108
H	0.78573801	-2.85223976	-2.75489164	C	1.24632645	1.34618012	3.13353406
H	1.51194743	-1.23479306	-2.46581319	H	1.32743463	4.50028048	1.82743050
H	-0.23452529	-1.35661682	-2.78748402	H	2.79859452	4.84557525	3.78268440
C	-0.70536668	-2.99198842	-0.63685585	H	3.28291344	2.96125419	5.34248309
H	-1.60575567	-2.68544174	-1.18113666	H	2.29549177	0.71113921	4.90844774
H	-0.93441722	-3.07082454	0.43331214	H	0.84610921	0.35270706	2.91802407
H	-0.37965029	-3.97799891	-1.01248172	C	-1.85822948	2.45992232	1.59608632
P	-0.20430349	2.08093284	0.86601627	C	-2.91070220	2.85369316	0.74922028

C	-4.18032191	3.11135624	1.27175282	C	-2.94883613	-0.62670224	0.91032109
C	-4.41604772	2.97907336	2.64476595	N	-4.26000279	-0.64230899	0.52409225
C	-3.37558961	2.58772187	3.49261911	H	-3.79577917	0.99569807	-4.23785882
C	-2.10293457	2.32847493	2.97285947	H	-5.90411820	0.56357987	-3.48707696
H	-2.73922421	2.97731184	-0.32141433	O	-1.53730622	0.54937749	-3.02115053
H	-4.98226739	3.42542706	0.60107403	H	-2.63089843	-0.85266340	1.92292180
H	-5.40544240	3.19481068	3.05315546	C	-5.42824369	-0.95407619	1.34097672
H	-3.54717036	2.49770617	4.56736062	H	-5.39830147	-1.99958206	1.67695635
H	-1.29440475	2.04283259	3.64795211	H	-6.31324326	-0.79943952	0.71235254
N	-3.84880069	0.55582651	-3.25565261	H	-5.47426973	-0.28465730	2.21009040
C	-5.10048344	0.33378920	-2.78016424	Cl	-5.18641676	2.71659402	-5.48842896
N	-5.39639256	-0.10100051	-1.56399526	O	-4.02932737	1.75626649	-5.63836775
C	-4.29095452	-0.25946179	-0.80820979	O	-6.41357453	1.92294226	-5.30192656
C	-2.96204723	-0.04418698	-1.17770646	O	-4.94363338	3.54107654	-4.29755142
C	-2.65387750	0.37198069	-2.52769492	O	-5.26847558	3.52807923	-6.69065132
N	-2.13904122	-0.27434339	-0.08650175				

Complex [Pt(PPh₃)(dmap)(NI-9mhy⁻)] (method A):

E = -2086.75409557 au

Pt	0.00000000	0.00000000	0.00000000	C	2.11732843	4.20673263	3.42859338
C	2.04322817	0.00000000	0.00000000	C	2.41105715	3.20297199	4.36558974
C	2.95825485	1.07862408	0.00000000	C	1.92643076	1.89966124	4.16818054
C	4.34904523	0.87570978	-0.06024913	C	1.15170979	1.60106460	3.03704559
C	4.87702633	-0.42183001	-0.13015037	H	1.11674963	4.70380310	1.57454174
C	3.99805201	-1.51589882	-0.14889550	H	2.50348378	5.22161686	3.57050585
C	2.61002663	-1.30844269	-0.08064332	H	3.02509842	3.43381075	5.24236691
H	2.59386775	2.10985069	0.04551666	H	2.16415691	1.10863836	4.88696502
H	5.02072378	1.74181922	-0.05567860	H	0.80480427	0.57812031	2.85111521
H	5.95906289	-0.58172629	-0.18232424	C	-1.94330718	2.62173282	1.26528440
H	4.39344158	-2.53711090	-0.21901705	C	-2.97869199	2.74796871	0.31139344
C	1.64057143	-2.46301252	-0.07887391	C	-4.27594219	3.08548293	0.72227245
H	1.37436650	-2.75502864	0.95422685	C	-4.55529907	3.29574763	2.08416287
H	2.04086805	-3.36254661	-0.59107840	C	-3.53267997	3.16373359	3.03528245
N	0.35926613	-2.03526720	-0.74146464	C	-2.22968559	2.82625687	2.63015121
C	0.54118392	-1.94464572	-2.22640431	H	-2.77130353	2.57867899	-0.75045454
H	0.70706951	-2.95899487	-2.64207361	H	-5.06968799	3.17992090	-0.02559490
H	1.41577286	-1.31398738	-2.43924629	H	-5.56942128	3.56001412	2.40163095
H	-0.35821010	-1.48223174	-2.66149475	H	-3.74334004	3.32466841	4.09773916
C	-0.71079841	-3.02530494	-0.44636539	H	-1.43671639	2.72811659	3.37790173
H	-1.62845746	-2.74402443	-0.97954612	N	-2.12925091	-0.33780025	-0.02835179
H	-0.91225773	-3.04182864	0.63494986	C	-2.79566853	-0.66408114	1.11200349
H	-0.38912573	-4.03188275	-0.77975422	N	-4.08569108	-0.98723677	1.24182786
P	-0.25358771	2.14560370	0.67946045	C	-4.72044347	-0.93938099	0.04159368
C	0.04555607	3.36570893	-0.67612261	C	-4.17955104	-0.61234497	-1.21705610
C	0.63900209	2.93077148	-1.87941078	C	-2.77001964	-0.28597814	-1.29961587
C	0.86366903	3.84063844	-2.92463865	N	-5.15803566	-0.67081385	-2.20265124
C	0.49566049	5.18724207	-2.78051641	C	-6.25584336	-1.02428599	-1.54957197
C	-0.11441073	5.62381885	-1.59232970	N	-6.06398481	-1.19976795	-0.18442704
C	-0.34734132	4.71778227	-0.54666875	H	-2.18861394	-0.65864650	2.02600616
H	0.89708280	1.87304913	-1.99335869	O	-2.11320338	0.00323145	-2.32614508
H	1.31591203	3.48989830	-3.85779140	H	-7.23820057	-1.16756740	-2.00226425
H	0.66807585	5.89430628	-3.59873613	C	-7.03300379	-1.62626581	0.81800142
H	-0.42259233	6.66890557	-1.48291758	H	-8.02207638	-1.20375942	0.58193345
H	-0.86103406	5.05714110	0.35894638	H	-6.70022477	-1.25617870	1.79898634
C	0.83879340	2.60969976	2.09998623	H	-7.10778865	-2.72660270	0.86161359
C	1.33085252	3.91542995	2.30217046				



Complex **[Pt(PPh₃)(dmap)(NI-9mhyp)]** (method B): $E = -2087.34906790$ au

Pt	0.00000000	0.00000000	0.00000000	C	2.20289048	4.14086854	3.38602612
C	2.04096974	0.00000000	0.00000000	C	2.43799938	3.15735759	4.35085242
C	2.95513429	1.07090769	0.00000000	C	1.89121145	1.88086879	4.18733042
C	4.33949689	0.86704704	-0.05319344	C	1.11434716	1.59046144	3.06366245
C	4.86343460	-0.42602420	-0.11618785	H	1.24903427	4.63157497	1.51747742
C	3.98472501	-1.51251448	-0.13367819	H	2.63790925	5.13591181	3.50006190
C	2.60248344	-1.30340056	-0.07287842	H	3.05556253	3.38182671	5.22286214
H	2.59674729	2.10080148	0.04341708	H	2.08244723	1.10252933	4.92873429
H	5.01061066	1.72952335	-0.04974275	H	0.71711900	0.58409209	2.91193706
H	5.94215715	-0.58781230	-0.16258914	C	-1.90781700	2.61470546	1.27354114
H	4.37748819	-2.53175265	-0.19863499	C	-2.94321341	2.73408320	0.32822459
C	1.63823490	-2.45478338	-0.07094090	C	-4.22947277	3.08845789	0.73594854
H	1.37506843	-2.74479589	0.95990351	C	-4.50061947	3.32371807	2.08874047
H	2.04462063	-3.35043554	-0.57776811	C	-3.47897619	3.20101297	3.03239487
N	0.36122690	-2.03843710	-0.73597267	C	-2.18674438	2.84727915	2.62861016
C	0.55170204	-1.95973387	-2.21541173	H	-2.74392709	2.54800340	-0.72918995
H	0.72889192	-2.97413414	-2.61750414	H	-5.02347259	3.17559621	-0.00803935
H	1.41962502	-1.32663455	-2.43190621	H	-5.50844815	3.60027604	2.40500778
H	-0.34550637	-1.51459563	-2.66423079	H	-3.68240145	3.38208033	4.08980532
C	-0.69544644	-3.03593961	-0.44283043	H	-1.39453955	2.76141848	3.37380311
H	-1.61216692	-2.77138421	-0.97992085	N	-2.11855236	-0.34745150	-0.03022909
H	-0.90078862	-3.05437178	0.63446712	C	-2.78923901	-0.67862227	1.09894802
H	-0.36096384	-4.03670787	-0.77027282	N	-4.06798167	-1.01911187	1.21567836
P	-0.23204907	2.12471534	0.68234981	C	-4.69250066	-0.99114035	0.01665501
C	0.06719320	3.35626772	-0.65259536	C	-4.14680375	-0.66205143	-1.23265432
C	0.65324727	2.94274122	-1.85900442	C	-2.74636165	-0.31266723	-1.30399601
C	0.87441806	3.86262057	-2.88785679	N	-5.11106757	-0.75059327	-2.22296397
C	0.51024694	5.20135516	-2.72431716	C	-6.20357464	-1.12164909	-1.58440861
C	-0.09160298	5.61869092	-1.53217390	N	-6.02178426	-1.28660927	-0.22133597
C	-0.31938417	4.70176239	-0.50400733	H	-2.19452462	-0.66102237	2.01812471
H	0.91246714	1.89101381	-1.99045260	O	-2.09206550	-0.01865891	-2.31919439
H	1.32162157	3.52547841	-3.82480363	H	-7.17422124	-1.29263059	-2.04707483
H	0.67892696	5.91776991	-3.53093622	C	-6.99606599	-1.68987915	0.77949069
H	-0.39732521	6.65935419	-1.40624946	H	-7.84958731	-0.99667076	0.79625779
H	-0.82551695	5.02941233	0.40612491	H	-6.49554003	-1.66888399	1.75564832
C	0.85932209	2.57863542	2.09753748	H	-7.36261884	-2.70866035	0.58497896
C	1.41404387	3.85659693	2.26715736				

Complex **[Pt(PPh₃)(dmap)(N3-9mhyp)]** (method A): $E = -2086.7283546$ au

Pt	0.00000000	0.00000000	0.00000000	C	2.14481781	4.32573282	3.33815315
C	2.04053795	0.00000000	0.00000000	C	2.65231397	3.34360834	4.20411660
C	2.94574536	1.08635917	0.00000000	C	2.29080377	1.99832698	4.02460053
C	4.33465403	0.89420386	-0.11541578	C	1.42523576	1.63574180	2.98141248
C	4.86703040	-0.39753436	-0.23960741	H	0.88179370	4.74087181	1.62785814
C	3.99533387	-1.49736758	-0.26496648	H	2.43171829	5.37448364	3.46717045
C	2.60889189	-1.30153122	-0.14672268	H	3.33560663	3.62508897	5.01195752
H	2.57565250	2.11222221	0.09314265	H	2.69481865	1.22633289	4.68749537
H	5.00136038	1.76385058	-0.10955711	H	1.17165121	0.58419967	2.81087338
H	5.94758817	-0.54816405	-0.33104118	C	-1.94614516	2.40378729	1.63646045
H	4.39467720	-2.51235832	-0.38284771	C	-3.11537030	2.49411656	0.84703142
C	1.64131553	-2.45739342	-0.17677967	C	-4.36766713	2.66241922	1.45536893
H	1.36974073	-2.77854346	0.84604958	C	-4.46845838	2.74640051	2.85465852
H	2.04343417	-3.34260571	-0.71090558	C	-3.31078881	2.66773070	3.64428836
N	0.35953551	-2.01135606	-0.83135096	C	-2.05309743	2.49552474	3.04119405
C	0.55150027	-1.88175901	-2.30839901	H	-3.05594562	2.42225027	-0.24295277
H	0.77389977	-2.87474085	-2.74709958	H	-5.26500089	2.71297852	0.83161512
H	1.38603680	-1.19535112	-2.50773057	H	-5.44850685	2.87127351	3.32587807
H	-0.37112803	-1.48455705	-2.75637553	H	-3.38070767	2.74300011	4.73454405
C	-0.71539953	-3.01016419	-0.57478248	H	-1.15602243	2.44164339	3.66550399
H	-1.64303991	-2.68870966	-1.06669060	N	-3.86173993	-0.05885230	-1.99478237
H	-0.89345444	-3.08993826	0.50728995	C	-2.63574716	0.07706345	-1.53581061
H	-0.41023585	-3.99846901	-0.97054971	N	-2.12441035	-0.26583324	-0.29895876
P	-0.31325592	2.10195687	0.82079822	C	-3.08400046	-0.80889513	0.51766356
C	-0.24144258	3.37902351	-0.51011248	C	-4.42595339	-1.01920474	0.15011010
C	0.43205064	3.08094533	-1.71435535	C	-4.88861727	-0.62703879	-1.18322648
C	0.51557740	4.04200756	-2.73380768	N	-5.12730250	-1.60225494	1.19899910
C	-0.07480098	5.30437178	-2.56309520	C	-4.23686704	-1.73616523	2.16420199
C	-0.75523587	5.60459728	-1.37144302	N	-2.96364553	-1.28200861	1.81951965
C	-0.84303485	4.64755671	-0.34853829	H	-1.89178124	0.53361199	-2.20682870
H	0.87463547	2.08778465	-1.84689857	O	-6.04759503	-0.74844994	-1.61021295
H	1.03450791	3.79863748	-3.66651333	H	-4.42580822	-2.15940604	3.15204006
H	-0.01580407	6.05019810	-3.36237819	C	-1.81416101	-1.22376799	2.71449796
H	-1.22961333	6.58247676	-1.23982802	H	-1.92050168	-0.40330096	3.44504237
H	-1.39976160	4.87869399	0.56532265	H	-0.90496435	-1.03387023	2.11139132
C	0.90045734	2.62028446	2.11691411	H	-1.70679908	-2.18098518	3.25174866
C	1.26843210	3.96914727	2.30050564				

Complex [Pt(PPh₃)(dmap)(N7-9mhyp)] (method A): E = -2086.74277707 au

Pt	0.00000000	0.00000000	0.00000000	C	-0.06418306	3.41709319	-0.33521327
C	2.03237064	0.00000000	0.00000000	C	0.28395264	3.07883839	-1.66024158
C	2.93493384	1.08680897	0.00000000	C	0.38339741	4.08372939	-2.63683152
C	4.32635192	0.89064201	-0.06782038	C	0.13707669	5.42327245	-2.30146888
C	4.86032688	-0.40418351	-0.14590812	C	-0.23675168	5.76259359	-0.98906314
C	3.98828710	-1.50385737	-0.18054860	C	-0.34925522	4.76470009	-0.01027898
C	2.59938579	-1.30503715	-0.10957828	H	0.42082506	2.02666108	-1.93284913
H	2.55985616	2.11442123	0.04292433	H	0.63283945	3.80681856	-3.66551570
H	4.99380966	1.75979654	-0.06423145	H	0.21254673	6.20338447	-3.06628227
H	5.94312576	-0.55735257	-0.20064850	H	-0.45689392	6.80359853	-0.73018147
H	4.38949919	-2.52082209	-0.27317662	H	-0.68838110	5.03144734	0.99635374
C	1.62171334	-2.45124446	-0.18046748	C	0.94834868	2.39501282	2.29998662
H	1.30751538	-2.77851827	0.82832180	C	1.51797372	3.65796832	2.55921988
H	2.03280307	-3.33400404	-0.71236304	C	2.37251496	3.83460154	3.65986212
N	0.37681500	-1.97413324	-0.88311666	C	2.65826183	2.75878473	4.51512103
C	0.63934336	-1.80127952	-2.34995109	C	2.09890208	1.49613882	4.25900568
H	0.77747022	-2.79633249	-2.81786207	C	1.25695670	1.31160588	3.15213483
H	1.55334723	-1.20479940	-2.47745760	H	1.31493919	4.50144345	1.89359008
H	-0.20142750	-1.25269170	-2.80521486	H	2.81882327	4.81739837	3.84433875
C	-0.72123693	-2.95901639	-0.70113138	H	3.32542258	2.90068754	5.37166522
H	-1.61278374	-2.61405542	-1.24325083	H	2.33241375	0.64766762	4.91052768
H	-0.95971668	-3.05290751	0.36899024	H	0.85580530	0.31913548	2.91665763
H	-0.41097668	-3.94517683	-1.09940785	C	-1.88622824	2.42783021	1.66591957
P	-0.22990374	2.06934871	0.91038754	C	-2.97092957	2.73370986	0.81314734

C	-4.24680991	2.96565166	1.34848471
C	-4.45501528	2.89683331	2.73755387
C	-3.38090060	2.59366679	3.58941618
C	-2.10088639	2.35887583	3.05816689
H	-2.82098908	2.78384572	-0.26992554
H	-5.07790623	3.20104477	0.67606535
H	-5.44980087	3.08811040	3.15365025
H	-3.53258772	2.54865607	4.67317536
H	-1.26735222	2.13282139	3.73060041
N	-3.72886837	0.37173978	-3.41912079
C	-4.94921153	0.09291521	-2.94085936
N	-5.33965255	-0.28694393	-1.68959454
C	-4.26722557	-0.35772874	-0.87975783
C	-2.93142665	-0.09438376	-1.21973639
C	-2.61102671	0.28746772	-2.58569618
N	-2.13190655	-0.27784771	-0.09102940
C	-2.95555420	-0.64005084	0.89883557
N	-4.25988094	-0.70994669	0.47422004
H	-5.77111088	0.18089044	-3.66527975
O	-1.43647568	0.51455880	-2.98998123
H	-2.65552614	-0.83115858	1.92690813
C	-5.44275970	-1.03627158	1.26487847
H	-5.32817697	-2.01888432	1.75046273
H	-6.29325160	-1.06887002	0.56781239
H	-5.62653232	-0.26366482	2.02935290

Table SI 2. Natural charges and HSAB-derived global and group parameters (in au) for the reaction of *N1*, *N3* or *N7* atoms in 9-mhypH derivatives with the Pt atom in [Pt(PPh₃)(dmab)]⁺.

	Pt	9-mhypH		9-mhypH·ClO ₄ ⁻		9-mhyp ⁻		
		<i>N3</i>	<i>N7</i>	<i>N3</i>	<i>N7</i>	<i>N1</i>	<i>N3</i>	<i>N7</i>
$A = E^N - E^{N+1}$ ^(a)	0.1476	-0.0183		-0.1203			-0.1780	
$I = E^{N-1} - E^N$ ^(b)	0.3805	0.3063		0.1755			0.1185	
$\mu = -\frac{1}{2}(I+A)$	-0.2640	-0.1440		-0.0276			0.0298	
$S = 1/(I-A)$	4.2927	3.0802		3.3815			3.3724	
$\omega = S \cdot \mu^2$	0.2993	0.0639		0.0026			0.0030	
q_M^{N+1} ^(c)	-0.2468	-	-	-	-	-	-	-
q_M^N ^(c)	0.0696	-0.0589	-0.2658	-0.1173	-0.3261	-0.1753	-0.2138	-0.4092
q_M^{N-1} ^(c)	-	0.1344	-0.0175	-0.0035	-0.1735	0.0296	-0.0304	-0.1935
$f^+ = q_M^{N+1} - q_M^N$	-0.3163	-	-	-	-	-	-	-
$f^- = q_M^N - q_M^{N-1}$	-	-0.1933	-0.2483	-0.1137	-0.1527	-0.2049	-0.1834	-0.2157
$s_{\pm} = S \cdot f^{\pm}$	-1.3579	-0.5953	-0.7648	-0.3846	-0.5163	-0.6912	-0.6184	-0.7273
$\Delta(s^2)_{kl} = (s_{k+} - s_{l-})^2$		0.58	0.35	0.95	0.71	0.44	0.55	0.40
$\Delta\Omega_{kl}$		3.8	2.9	11.4	6.7	20.0	29.5	11.5

^(a) Electron affinity (au); ^(b) Vertical ionization potential (au); ^(c) Mulliken group charges (in e) after summation over all neighbouring atoms.