

SUPPORTING INFORMATION

**Oxidative Addition of Dihydrogen to (η^6 -Arene)Mo(PMe₃)₃ Complexes:
Origin of The Naphthalene and Anthracene Effects**

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Computational data for geometry optimized structures.

Table S1. Cartesian Coordinated for Geometry Optimized Structures

(PhH)Mo(PH₃)₃
(-1329.433828769540 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
Mo1	-0.04911	-0.04047	0.016929
P2	1.827395	0.660735	-1.32844
P3	-0.19207	-2.0405	-1.32473
P4	-1.55892	1.05882	-1.50916
C5	-1.55455	-0.1382	1.806296
C6	-0.70762	-1.27327	1.862014
H7	-1.14198	-2.26757	1.852328
C8	0.712484	-1.12348	1.946872
H9	1.354408	-1.9943	2.008715
C10	1.274056	0.177314	1.903837
H11	2.352016	0.297856	1.933257
C12	0.435258	1.335529	1.847731
C13	-0.97007	1.167682	1.763839
H14	-2.62997	-0.26405	1.765151
H15	0.868925	2.328326	1.832592
H16	-1.61161	2.039155	1.684287
H17	2.996506	1.195086	-0.70812
H18	2.538831	-0.24917	-2.17075
H19	-0.34046	-3.31498	-0.69919

H20	-1.23091	-2.25171	-2.28386
H21	-2.65262	1.825734	-1.00625
H22	-1.12502	2.05571	-2.43688
H23	1.733703	1.688049	-2.31817
H24	0.862425	-2.45188	-2.19824
H25	-2.34103	0.340048	-2.46588

(NpH)Mo(PH₃)₃

(-1483.111463278280 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
Mo1	2.337754	-0.19371	0.001846
P2	1.919373	-0.61814	-2.34277
P3	4.496644	-1.14724	-0.25601
P4	1.48191	-2.37652	0.60267
H5	1.368347	0.393431	-3.18467
H6	1.030956	-1.64374	-2.79078
H7	2.977173	-0.96643	-3.23711
H8	5.632152	-0.48139	0.298985
H9	5.096223	-1.37572	-1.53646
H10	4.841334	-2.4368	0.262528
H11	0.63058	-2.53751	1.735766
H12	2.354625	-3.4544	0.943166
H13	0.661473	-3.14976	-0.27511

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C14	1.836095	0.643256	2.102537
C15	3.108381	1.137202	1.731074
C16	3.260599	1.868777	0.513671
C17	2.138955	2.087882	-0.31941
C18	0.803648	1.746058	0.12501
C19	-0.36513	2.071861	-0.62306
C20	-1.62122	1.722614	-0.17627
C21	-1.772	1.000882	1.033529
C22	-0.66428	0.643374	1.771114
C23	0.649968	1.010318	1.357808
H24	1.722175	0.077356	3.021156
H25	3.971978	0.9316	2.353782
H26	4.239963	2.219708	0.20823
H27	2.255582	2.630614	-1.25163
H28	-0.24705	2.635745	-1.54494
H29	-2.49896	1.999858	-0.75287
H30	-2.7649	0.727613	1.379049
H31	-0.77839	0.099973	2.705654

(AnH)Mo(PH₃)₃

(-1636.792079728550 Hartree)

atom

x

y

z

Mo1	1.154736	0.304974	0.852561
P2	0.894085	0.807024	-1.50295
P3	3.380667	-0.35048	0.392131
P4	0.471175	-2.00439	0.56043
H5	0.35778	2.057843	-1.93278
H6	0.087024	0.022867	-2.38306
H7	2.026265	0.847691	-2.37326
H8	4.44239	0.12162	1.223922
H9	4.038881	-0.04246	-0.84291
H10	3.804176	-1.71887	0.409783
H11	-0.37447	-2.6443	1.514901
H12	1.439158	-3.05264	0.51517
H13	-0.26566	-2.46145	-0.57448
C14	0.552135	0.267793	3.096778
C15	1.796881	0.928642	2.981511
C16	1.920782	2.072321	2.135601
C17	0.798022	2.525532	1.405938
C18	-0.53345	2.009974	1.674803
C19	-1.68802	2.533839	1.07495
C20	-2.96184	1.986644	1.300164
C21	-4.14149	2.528629	0.705071
C22	-3.08688	0.834397	2.16218
C23	-4.38612	0.284244	2.384747

C24	-1.93224	0.293917	2.751003
C25	-0.65919	0.84712	2.544405
C26	-5.49707	0.834575	1.794169
C27	-5.3735	1.970691	0.943558
H28	0.463925	-0.6105	3.727735
H29	2.664479	0.544253	3.50677
H30	2.88163	2.560463	2.015656
H31	0.896203	3.377842	0.741304
H32	-1.59467	3.407261	0.433236
H33	-4.04433	3.395879	0.05652
H34	-4.47842	-0.58282	3.034259
H35	-2.02886	-0.56768	3.407997
H36	-6.47872	0.405096	1.973265
H37	-6.26223	2.394054	0.484252

(1,2-Me₂C₆H₄)Mo(PH₃)₃
 (-1408.08965810614 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
Mo1	0.885118	0.260675	0.142081
P2	0.143325	0.818956	-2.08393
P3	3.062515	-0.25786	-0.74977
P4	0.214655	-2.02336	-0.24988
H5	-0.68731	1.955852	-2.31869

H6	-0.64462	-0.07553	-2.8767
H7	1.063723	1.12681	-3.13349
H8	4.226363	0.216014	-0.07107
H9	3.493967	0.165739	-2.04616
H10	3.543429	-1.59646	-0.90027
H11	-0.569	-2.73544	0.707412
H12	1.168168	-3.07367	-0.42624
H13	-0.58772	-2.40271	-1.37301
C14	0.644214	0.062202	2.441771
C15	1.836188	0.779869	2.193371
C16	1.787407	1.979211	1.415708
C17	0.54728	2.424978	0.905044
C18	-0.67359	1.706895	1.155317
C19	-1.97813	2.305089	0.685253
C20	-1.87299	-0.23705	2.334903
C21	-0.62408	0.510457	1.932485
H22	0.680722	-0.84935	3.029238
H23	2.780063	0.418532	2.58624
H24	2.693109	2.539165	1.211335
H25	0.509077	3.330244	0.30786
H26	-2.70038	1.546715	0.374821
H27	-1.81511	2.973589	-0.16515
H28	-2.44601	2.899534	1.482133

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H29	-2.62646	-0.25266	1.544217
H30	-2.33407	0.220761	3.220915
H31	-1.63979	-1.27487	2.589956

(PhH)Mo(PH₃)₃H₂
(-1330.579934888850 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
C1	-0.24618	0.198337	0.799811
C2	0.382412	-0.25296	1.994442
C3	1.851483	-0.38446	1.997901
C4	1.492055	-1.08975	-0.26626
C5	0.343146	-0.23709	-0.42408
C6	2.415302	-0.79773	0.846834
H7	-1.12175	0.838321	0.814849
H8	-0.11706	-0.04422	2.935506
H9	2.417553	-0.11664	2.885112
H10	1.920966	-1.51261	-1.17135
H11	-0.02664	0.091966	-1.38949
H12	3.488047	-0.90093	0.707983
Mo13	-0.56821	-2.08094	0.583667
P14	-2.7754	-1.36608	-0.2169
P15	0.8172	-3.56417	1.922784

P16	-0.42877	-3.56952	-1.3548
H17	-1.59552	-3.47601	0.773145
H18	-1.48666	-2.18099	2.014281
H19	-3.00355	-0.04422	-0.6987
H20	-3.42466	-2.02929	-1.29891
H21	-3.88864	-1.40731	0.658776
H22	2.094354	-3.13064	2.375989
H23	0.321198	-4.02868	3.165227
H24	1.223864	-4.84263	1.442597
H25	0.050909	-4.90029	-1.21354
H26	-1.58002	-3.90797	-2.11772
H27	0.40164	-3.21335	-2.45176

(NpH)Mo(PH₃)₃H₂

(-1484.289273645170 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
Mo1	0.00204	0.19951	0.221644
P2	-2.35391	0.22067	0.908957
P3	2.345743	0.671225	0.732154
P4	0.187227	-2.0584	1.164861
C5	2.88606	-0.35388	-3.15658
C6	2.337077	2.383697	-2.92908

C7	3.761931	0.589277	-3.71913
C8	3.489435	1.951153	-3.60518
C9	1.46333	1.451736	-2.36956
C10	0.228758	1.787951	-1.63464
H11	0.042199	2.837679	-1.43047
C12	-0.89744	0.929594	-1.76132
H13	-1.91258	1.311284	-1.77329
C14	-0.62554	-0.46963	-1.86536
H15	-1.41801	-1.19861	-1.99342
C16	0.767753	-0.82006	-1.8155
H17	1.012464	-1.88007	-1.80561
C18	1.741494	0.068939	-2.48186
H19	0.008019	0.226316	1.963905
H20	-0.11256	1.737058	0.945441
H21	-3.40302	0.138348	-0.04961
H22	-2.8783	-0.76984	1.787711
H23	3.279811	0.895014	-0.31151
H24	2.661889	1.804623	1.517785
H25	1.31864	-2.42074	1.945708
H26	-0.78433	-2.56026	2.072358
H27	3.101501	-1.4168	-3.24178
H28	2.123797	3.446379	-2.83775
H29	4.65754	0.252879	-4.23423

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H30	4.170692	2.682191	-4.03181
H31	-2.87553	1.330149	1.618714
H32	3.132541	-0.2527	1.476036
H33	0.216192	-3.19265	0.309444

(AnH)Mo(PH₃)₃H₂

(most stable geometry, -1637.978433930750 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
Mo1	-0.01203	0.190553	0.223757
P2	-2.35893	0.237951	0.938487
P3	2.331904	0.69204	0.741411
P4	0.162514	-2.09281	1.104067
C5	2.893721	-0.29308	-3.06816
C6	2.260459	2.440152	-2.83993
C7	3.799929	0.673289	-3.60449
C8	5.014507	0.304427	-4.23582
H9	5.259278	-0.75196	-4.32067
C10	5.876332	1.261599	-4.73796
H11	6.801915	0.960939	-5.22125
C12	5.556692	2.633867	-4.62495
H13	6.237733	3.381573	-5.02222
C14	4.38157	3.024215	-4.01077

H15	4.134097	4.079527	-3.92071
C16	3.476924	2.066028	-3.48774
C17	1.404564	1.489235	-2.33355
C18	0.147973	1.782308	-1.62396
H19	-0.07149	2.826103	-1.42292
C20	-0.95044	0.889384	-1.75255
H21	-1.97628	1.241937	-1.76617
C22	-0.63935	-0.50148	-1.855
H23	-1.41276	-1.25183	-1.97525
C24	0.760606	-0.81928	-1.81348
H25	1.030787	-1.87295	-1.81259
C26	1.726072	0.093149	-2.45132
H27	0.012369	0.185897	1.962877
H28	-0.11597	1.728124	0.947288
H29	-3.40783	-0.05487	0.025319
H30	-2.82603	-0.59985	1.985425
H31	-2.92345	1.436827	1.444391
H32	3.316194	0.696376	-0.28203
H33	2.651527	1.94255	1.32069
H34	3.046642	-0.10604	1.675111
H35	1.340198	-2.54991	1.767666
H36	-0.75447	-2.58201	2.077022
H37	0.051408	-3.18785	0.194505

H38	3.145981	-1.34851	-3.14982
H39	2.01947	3.497054	-2.74693

(AnH)Mo(PH₃)₃H₂

(second most stable geometry, -1637.97519036198 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
Mo1	0.100124	-0.03737	-0.29053
P2	2.17597	0.015742	-1.59509
P3	-1.39638	-1.91349	0.222044
P4	1.274899	-0.13631	1.885321
C5	0.680878	3.925605	1.59407
C6	-1.55901	2.693065	2.770642
C7	0.239885	4.376122	2.877091
C8	0.899836	5.411732	3.584225
H9	1.766348	5.885603	3.128456
C10	0.457948	5.818897	4.829524
H11	0.975004	6.615958	5.356811
C12	-0.66666	5.200402	5.420116
H13	-1.0095	5.524564	6.398913
C14	-1.32949	4.185499	4.754941
H15	-2.19439	3.706657	5.208572
C16	-0.90168	3.74802	3.476861

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C17	-1.10913	2.275585	1.540616
C18	-1.67211	1.159487	0.756586
H19	-2.48726	0.617917	1.232036
C20	-1.70329	1.250387	-0.68429
H21	-2.52209	0.87144	-1.28387
C22	-0.57243	1.872747	-1.27831
H23	-0.48865	1.989128	-2.35205
C24	0.440214	2.322864	-0.35378
H25	1.353399	2.728382	-0.78398
C26	0.033388	2.904452	0.939939
H27	0.883415	-1.58597	-0.40827
H28	-0.29445	-0.7379	-1.81175
H29	2.47249	1.169487	-2.36503
H30	3.454497	-0.10158	-0.98245
H31	2.391927	-0.94406	-2.60709
H32	-2.79311	-1.67238	0.273004
H33	-1.43251	-3.03622	-0.63219
H34	-1.31452	-2.63907	1.443147
H35	0.991222	-1.15013	2.840115
H36	2.687566	-0.27289	1.960382
H37	1.157685	0.969251	2.763405
H38	1.550299	4.400861	1.143311
H39	-2.42121	2.213338	3.230445

H₂

(-1.179997313330 Hartree)

<u>atom</u>	<u>x</u>	<u>y</u>	<u>z</u>
H1	0	0	0.371283125
H2	0	0	-0.371283125