Electronic Supplementary Material (ESI) for Dalton Transactions

What is the best bonding model of the (σ-H-BR) Species bound to a transition metal?: Bonding analysis in complexes $[(H)_2Cl(PMe_3)_2M(\sigma\text{-H-BR})]$ (M = Fe, Ru, Os)

Krishna K. Pandey

School of Chemical Sciences, Devi Ahilya University Indore, Khandwa Road Campus, Indore 452017, India

E-mail: kkpandey.schem@dauniv.ac.in

Supporting Information

Cartesian coordinates of terminal neutral complexes of iron, ruthenium and osmium $[(H)_2Cl(PMe_3)_2M(\sigma\text{-H-BR})]$ (M = Fe, **I**, R = OMe, **II**, R = NMe_2, **III**, R = Ph; M = Ru, **IV**, R = OMe, **V**, R = NMe_2, **VI**, R = Ph; M = Os, **VII**, R = OMe, **VIII**, R = NMe_2, **IX**, R = Ph)

$[(H)_2Cl(PMe_3)_2Fe(HBOMe)]$ (**I**)

B	-1.796598	0.412352	0.000000
H	-0.982060	1.415364	0.000000
O	-3.143526	0.527238	0.000000
C	-3.769162	1.821967	0.000000
H	-3.485067	2.391816	0.894772
H	-3.485067	2.391816	-0.894772
H	-4.851989	1.661122	0.000000
Fe	-0.058034	-0.032264	0.000000
Cl	1.893764	1.245229	0.000000
P	0.318240	-0.303639	-2.159284
P	0.318240	-0.303639	2.159284
C	-0.812467	-1.435971	-3.085994
C	-0.812467	-1.435971	3.085994
C	0.303806	1.205827	-3.226450
C	0.303806	1.205827	3.226450
C	1.964519	-1.025135	-2.568754
C	1.964519	-1.025135	2.568754
H	0.612440	-1.379372	0.000000
H	-1.356394	-0.902150	0.000000
H	-1.839013	-1.045628	-3.055924
H	-0.494935	-1.538859	-4.133621
H	-0.805385	-2.424879	-2.607841
H	-0.494935	-1.538859	4.133621
H	-1.839013	-1.045628	3.055924
H	-0.805385	-2.424879	2.607841
H	-0.702109	1.647796	-3.226671

H	1.007437	1.932417	-2.798556
H	0.597354	0.967525	-4.259213
H	1.007437	1.932417	2.798556
H	-0.702109	1.647796	3.226671
H	0.597354	0.967525	4.259213
H	2.739562	-0.402324	2.104384
H	2.113321	-1.066606	3.657360
H	2.028811	-2.037510	2.148686
H	2.113321	-1.066606	-3.657360
H	2.739562	-0.402324	-2.104384
H	2.028811	-2.037510	-2.148686

$[(H)_2Cl(PMe_3)_2Fe(HBNMe_2)]$ (II)

B	1.690051	0.344560	0.000000
N	3.088645	0.460775	0.000000
C	3.760766	1.755497	0.000000
C	3.988053	-0.686265	0.000000
H	3.018607	2.560960	0.000000
H	0.927761	1.366679	0.000000
H	4.400192	1.869380	0.891449
H	4.400192	1.869380	-0.891449
H	4.638283	-0.680316	0.891026
H	4.638283	-0.680316	-0.891026
H	3.409221	-1.616266	0.000000
Fe	-0.094231	-0.048123	0.000000
Cl	-2.015413	1.271616	0.000000
P	-0.449577	-0.278291	-2.165095
P	-0.449577	-0.278291	2.165095
C	0.666934	-1.413287	3.110472
C	0.666934	-1.413287	-3.110472
C	-0.392280	1.247548	3.208626
C	-0.392280	1.247548	-3.208626
C	-2.104119	-0.961182	2.610248
C	-2.104119	-0.961182	-2.610248
H	-0.816334	-1.365565	0.000000
H	1.203073	-0.936942	0.000000
H	1.698688	-1.037836	3.068196
H	0.354792	-1.490420	4.162049
H	0.641134	-2.411821	2.653056
H	0.354792	-1.490420	-4.162049
H	1.698688	-1.037836	-3.068196
H	0.641134	-2.411821	-2.653056
H	0.620784	1.672099	3.181983
H	-1.091152	1.978802	2.780922
H	-0.670725	1.032073	4.250637
H	-1.091152	1.978802	-2.780922
H	0.620784	1.672099	-3.181983
H	-0.670725	1.032073	-4.250637
H	-2.872836	-0.331975	-2.143964
H	-2.240909	-0.981121	-3.701017

H	-2.193336	-1.979027	-2.208316
H	-2.240909	-0.981121	3.701017
H	-2.872836	-0.331975	2.143964
H	-2.193336	-1.979027	2.208316

[$(H)_2Cl(PMe_3)_2Fe(HBPh)$] (III)

B	1.309220	-0.181320	0.000000
H	0.646015	-1.279066	0.000000
C	2.845308	-0.142119	0.000000
C	3.560576	1.075089	0.000000
C	3.591311	-1.341506	0.000000
C	4.953986	1.094688	0.000000
C	4.984823	-1.325460	0.000000
C	5.669635	-0.106600	0.000000
H	3.009480	2.016646	0.000000
H	3.062826	-2.295711	0.000000
H	5.486468	2.045788	0.000000
H	5.540672	-2.263053	0.000000
H	6.759569	-0.092796	0.000000
Fe	-0.483761	0.000871	0.000000
Cl	-2.243307	-1.534257	0.000000
P	-0.911519	0.216288	-2.159802
P	-0.911519	0.216288	2.159802
C	0.047496	1.497138	-3.083742
C	0.047496	1.497138	3.083742
C	-0.673427	-1.281755	-3.211639
C	-0.673427	-1.281755	3.211639
C	-2.644075	0.694344	-2.565370
C	-2.644075	0.694344	2.565370
H	-1.358060	1.224479	0.000000
H	0.675255	1.041536	0.000000
H	1.117759	1.251264	-3.055353
H	-0.283485	1.554721	-4.130695
H	-0.098420	2.475332	-2.605496
H	-0.283485	1.554721	4.130695
H	1.117759	1.251264	3.055353
H	-0.098420	2.475332	2.605496
H	0.386163	-1.571166	-3.200585
H	-1.267954	-2.099194	-2.782536
H	-0.991332	-1.093519	-4.247481
H	-1.267954	-2.099194	2.782536
H	0.386163	-1.571166	3.200585
H	-0.991332	-1.093519	4.247481
H	-3.322666	-0.029972	2.097704
H	-2.797695	0.709432	3.653903
H	-2.850488	1.689623	2.150363
H	-2.797695	0.709432	-3.653903
H	-3.322666	-0.029972	-2.097704
H	-2.850488	1.689623	-2.150363

$[(H)_2Cl(PMe_3)_2Ru(HBOMe)]$ (IV)

B	-1.857998	0.398509	0.000000
H	-1.159773	1.490535	0.000000
O	-3.205441	0.353695	0.000000
C	-3.979466	1.566894	0.000000
H	-3.764049	2.166021	0.894309
H	-3.764049	2.166021	-0.894309
H	-5.035879	1.280000	0.000000
Ru	-0.021245	-0.100191	0.000000
Cl	2.117141	1.139104	0.000000
P	0.302727	-0.246245	-2.320685
P	0.302727	-0.246245	2.320685
C	-0.903258	-1.204643	-3.341314
C	-0.903258	-1.204643	3.341314
C	0.401751	1.357562	-3.229518
C	0.401751	1.357562	3.229518
C	1.900293	-1.033219	-2.789946
C	1.900293	-1.033219	2.789946
H	0.700435	-1.532834	0.000000
H	-1.263838	-1.150174	0.000000
H	-1.900903	-0.751068	-3.262835
H	-0.597077	-1.227228	-4.397117
H	-0.962509	-2.232230	-2.958145
H	-0.597077	-1.227228	4.397117
H	-1.900903	-0.751068	3.262835
H	-0.962509	-2.232230	2.958145
H	-0.564260	1.877613	-3.169874
H	1.163848	1.976513	-2.736933
H	0.669925	1.203628	-4.284797
H	1.163848	1.976513	2.736933
H	-0.564260	1.877613	3.169874
H	0.669925	1.203628	4.284797
H	2.707576	-0.497234	2.273261
H	2.053006	-0.993179	3.878197
H	1.902176	-2.078726	2.454203
H	2.053006	-0.993179	-3.878197
H	2.707576	-0.497234	-2.273261
H	1.902176	-2.078726	-2.454203

$[(H)_2Cl(PMe_3)_2Ru(HBNMe_2)]$ (V)

B	1.747011	0.392580	0.000000
N	3.147551	0.347792	0.000000
C	3.960291	1.560537	0.000000
C	3.921350	-0.888417	0.000000
H	3.312138	2.442917	0.000000
H	1.109504	1.493191	0.000000
H	4.608769	1.602376	0.891088
H	4.608769	1.602376	-0.891088

H	4.568885	-0.949320	0.891067
H	4.568885	-0.949320	-0.891067
H	3.245649	-1.750183	0.000000
Ru	-0.123234	-0.102997	0.000000
Cl	-2.251981	1.137498	0.000000
P	-0.412999	-0.218981	-2.322168
P	-0.412999	-0.218981	2.322168
C	0.789797	-1.180199	3.347678
C	0.789797	-1.180199	-3.347678
C	-0.466939	1.398515	-3.212816
C	-0.466939	1.398515	3.212816
C	-2.016643	-0.970537	-2.832429
C	-2.016643	-0.970537	2.832429
H	-0.834145	-1.531396	0.000000
H	1.115865	-1.151269	0.000000
H	1.793111	-0.743745	3.246527
H	0.499081	-1.176107	4.408157
H	0.824999	-2.216805	2.985990
H	0.499081	-1.176107	-4.408157
H	1.793111	-0.743745	-3.246527
H	0.824999	-2.216805	-2.985990
H	0.503898	1.904258	3.117675
H	-1.234368	2.021534	2.733676
H	-0.706944	1.263723	4.277526
H	-1.234368	2.021534	-2.733676
H	0.503898	1.904258	-3.117675
H	-0.706944	1.263723	-4.277526
H	-2.822736	-0.429893	-2.318825
H	-2.152414	-0.909908	-3.921953
H	-2.042483	-2.021437	-2.514734
H	-2.152414	-0.909908	3.921953
H	-2.822736	-0.429893	2.318825
H	-2.042483	-2.021437	2.514734

$[(H)_2Cl(PMe_3)_2Ru(HBPh)]$ (VI)

B	1.359775	-0.262431	0.000000
H	0.761800	-1.401473	0.000000
C	2.891399	-0.120376	0.000000
C	3.529912	1.137942	0.000000
C	3.708651	-1.271597	0.000000
C	4.919674	1.242385	0.000000
C	5.099033	-1.171392	0.000000
C	5.707463	0.086907	0.000000
H	2.919670	2.042128	0.000000
H	3.238434	-2.255479	0.000000
H	5.393527	2.224022	0.000000
H	5.711024	-2.073310	0.000000
H	6.794602	0.167492	0.000000
Ru	-0.520265	0.048314	0.000000

Cl	-2.526702	-1.398411	0.000000
P	-0.875805	0.155661	-2.323458
P	-0.875805	0.155661	2.323458
C	0.207252	1.252175	-3.339720
C	0.207252	1.252175	3.339720
C	-0.773470	-1.452742	-3.219426
C	-0.773470	-1.452742	3.219426
C	-2.557017	0.744263	-2.788077
C	-2.557017	0.744263	2.788077
H	-1.393063	1.395831	0.000000
H	0.610257	1.212567	0.000000
H	1.251609	0.921662	-3.256562
H	-0.096779	1.234853	-4.396261
H	0.137769	2.280288	-2.959516
H	-0.096779	1.234853	4.396261
H	1.251609	0.921662	3.256562
H	0.137769	2.280288	2.959516
H	0.250709	-1.844526	-3.154000
H	-1.453342	-2.159281	-2.724557
H	-1.056368	-1.339199	-4.275916
H	-1.453342	-2.159281	2.724557
H	0.250709	-1.844526	3.154000
H	-1.056368	-1.339199	4.275916
H	-3.294344	0.115701	2.271488
H	-2.702934	0.685556	3.876367
H	-2.683698	1.782445	2.453504
H	-2.702934	0.685556	-3.876367
H	-3.294344	0.115701	-2.271488
H	-2.683698	1.782445	-2.453504

[$(H)_2Cl(PMe_3)_2Os(HBOMe)$] (VII)

B	-1.830260	0.413532	0.000000
H	-1.018117	1.464886	0.000000
O	-3.173312	0.456664	0.000000
C	-3.886243	1.706299	0.000000
H	-3.642082	2.293387	0.894801
H	-3.642082	2.293387	-0.894801
H	-4.955262	1.471475	0.000000
Os	0.007401	-0.149007	0.000000
Cl	2.108890	1.194020	0.000000
P	0.284817	-0.262927	-2.335341
P	0.284817	-0.262927	2.335341
C	-0.908319	-1.264276	-3.325826
C	-0.908319	-1.264276	3.325826
C	0.286951	1.344792	-3.242406
C	0.286951	1.344792	3.242406
C	1.903394	-0.976017	-2.848080
C	1.903394	-0.976017	2.848080
H	0.875064	-1.537972	0.000000

H	-1.015864	-1.411202	0.000000
H	-1.921083	-0.854796	-3.208809
H	-0.635676	-1.262480	-4.391049
H	-0.910425	-2.296776	-2.951527
H	-0.635676	-1.262480	4.391049
H	-1.921083	-0.854796	3.208809
H	-0.910425	-2.296776	2.951527
H	-0.700536	1.818925	-3.155089
H	1.033262	1.999703	-2.772126
H	0.531040	1.204731	-4.305284
H	1.033262	1.999703	2.772126
H	-0.700536	1.818925	3.155089
H	0.531040	1.204731	4.305284
H	2.699657	-0.402663	2.354508
H	2.026246	-0.932538	3.939828
H	1.962328	-2.019200	2.510231
H	2.026246	-0.932538	-3.939828
H	2.699657	-0.402663	-2.354508
H	1.962328	-2.019200	-2.510231

$[(H)_2Cl(PMe_3)_2Os(HBNMe_2)]$ (VIII)

B	1.689801	0.459013	0.000000
N	3.086764	0.537380	0.000000
C	3.805576	1.806452	0.000000
C	3.940454	-0.645327	0.000000
H	0.908653	1.494284	0.000000
H	3.094444	2.638745	0.000000
H	4.448964	1.897394	0.891200
H	4.448964	1.897394	-0.891200
H	4.590445	-0.663763	0.891386
H	4.590445	-0.663763	-0.891386
H	3.320067	-1.547373	0.000000
Os	-0.159288	-0.145638	0.000000
Cl	-2.236257	1.220064	0.000000
P	-0.394313	-0.259726	2.335856
P	-0.394313	-0.259726	-2.335856
C	0.684765	-1.431555	3.273304
C	0.684765	-1.431555	-3.273304
C	-0.164396	1.310275	3.282895
C	-0.164396	1.310275	-3.282895
C	-2.071998	-0.780551	2.895889
C	-2.071998	-0.780551	-2.895889
H	-0.997039	-1.549095	0.000000
H	0.882227	-1.396974	0.000000
H	1.740256	-1.189903	3.088556
H	0.483441	-1.381734	4.353455
H	0.495703	-2.452500	2.914904
H	0.483441	-1.381734	-4.353455
H	1.740256	-1.189903	-3.088556

H	0.495703	-2.452500	-2.914904
H	0.824061	1.735952	3.062247
H	-0.932305	2.024481	2.954544
H	-0.258731	1.141276	4.365404
H	-0.932305	2.024481	-2.954544
H	0.824061	1.735952	-3.062247
H	-0.258731	1.141276	-4.365404
H	-2.815003	-0.184595	-2.349474
H	-2.190241	-0.635319	-3.979240
H	-2.220534	-1.840492	-2.649258
H	-2.190241	-0.635319	3.979240
H	-2.815003	-0.184595	2.349474
H	-2.220534	-1.840492	2.649258

$[(H)_2Cl(PMe_3)_2Os(HBPh)]$ (IX)

B	1.333990	-0.253743	0.000000
H	0.665933	-1.378143	0.000000
C	2.867624	-0.154493	0.000000
C	3.524736	1.094226	0.000000
C	3.666220	-1.318196	0.000000
C	4.916116	1.176550	0.000000
C	5.058076	-1.239073	0.000000
C	5.686190	0.009357	0.000000
H	2.927519	2.006622	0.000000
H	3.182814	-2.295440	0.000000
H	5.404850	2.150895	0.000000
H	5.655903	-2.150453	0.000000
H	6.774424	0.073035	0.000000
Os	-0.552113	0.096558	0.000000
Cl	-2.484124	-1.477922	0.000000
P	-0.859405	0.172530	-2.339186
P	-0.859405	0.172530	2.339186
C	0.189284	1.325155	-3.325188
C	0.189284	1.325155	3.325188
C	-0.642995	-1.424307	-3.234735
C	-0.642995	-1.424307	3.234735
C	-2.560408	0.663718	-2.842007
C	-2.560408	0.663718	2.842007
H	-1.553979	1.393155	0.000000
H	0.350066	1.447174	0.000000
H	1.246528	1.050781	-3.208305
H	-0.081445	1.288305	-4.390238
H	0.052941	2.348378	-2.950007
H	-0.081445	1.288305	4.390238
H	1.246528	1.050781	3.208305
H	0.052941	2.348378	2.950007
H	0.400227	-1.756385	-3.142491
H	-1.294379	-2.172193	-2.762244
H	-0.902174	-1.323369	-4.298426

H	-1.294379	-2.172193	2.762244
H	0.400227	-1.756385	3.142491
H	-0.902174	-1.323369	4.298426
H	-3.271966	-0.010525	2.346982
H	-2.678454	0.604245	3.933413
H	-2.756320	1.689929	2.504021
H	-2.678454	0.604245	-3.933413
H	-3.271966	-0.010525	-2.346982
H	-2.756320	1.689929	-2.504021