

Supporting Information
for

**‘Ruthenium trihydrides with *N*-heterocyclic carbene ligands:
effects on quantum mechanical exchange coupling’**

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Coordinates for the optimised geometry of [CpRuH*₃(IMes)] 1**

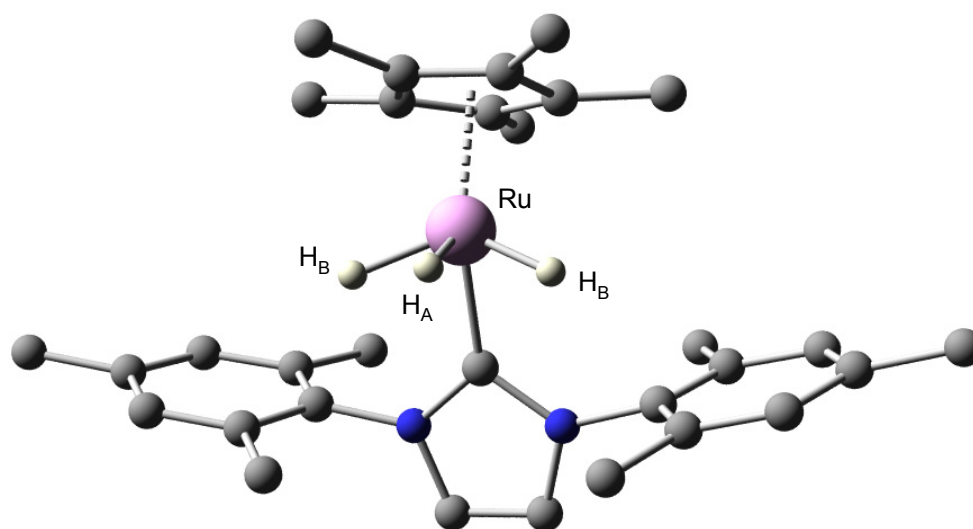
(atom, x-, y-, z-positions in Å)

Ru	-0.005481	0.923878	-0.590584
N	-1.083411	-1.906586	0.180232
N	1.073507	-1.908650	0.178811
C	-1.126208	2.585138	0.664939
C	0.075696	2.348184	1.402845
C	1.189573	2.624757	0.552107
C	0.677268	3.081867	-0.719845
C	-0.754359	3.059210	-0.649640
C	0.151502	2.015995	2.866717
C	2.635578	2.636614	0.964434
C	1.501752	3.653582	-1.841113
C	-1.700819	3.608349	-1.682243
C	-2.522091	2.564000	1.224253
C	-0.004278	-1.059039	-0.018057
C	-0.680999	-3.205913	0.483720
C	0.668912	-3.207199	0.482958
C	-2.483383	-1.583164	0.078082
C	-3.127814	-1.710837	-1.164990
C	-4.500090	-1.451247	-1.220634
C	-5.233424	-1.084545	-0.086728
C	-4.561956	-0.999569	1.136116
C	-3.189826	-1.251053	1.244048
C	2.473960	-1.587808	0.076341
C	3.183376	-1.266398	1.243704
C	4.556180	-1.018282	1.135510
C	5.225736	-1.096948	-0.088756
C	4.489793	-1.454434	-1.223825
C	3.116770	-1.710506	-1.168131
C	-2.368631	-2.113772	-2.405169
C	-6.709439	-0.775396	-0.186511
C	-2.500937	-1.193053	2.586497
C	2.499743	-1.222867	2.589555
C	6.702559	-0.791780	-0.188141
C	2.356783	-2.109137	-2.409284
H	-0.027901	0.625173	-2.149022
H	1.374896	0.409365	-1.181527
H	-1.396103	-3.992974	0.664882
H	-1.402473	0.416527	-1.144883
H	1.382645	-3.995639	0.663487
H	-5.009498	-1.541647	-2.177842
H	-5.118235	-0.735582	2.033254
H	5.114712	-0.763298	2.033900
H	4.997881	-1.541420	-2.182036
H	-3.046287	-2.208731	-3.259071
H	-1.604208	-1.367584	-2.648407
H	-1.855098	-3.073670	-2.271485
H	-7.218895	-0.934565	0.769798
H	-6.876587	0.271054	-0.474744

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H	-7.200213	-1.400182	-0.940867
H	-1.578721	-0.606880	2.535507
H	-3.156009	-0.746138	3.340680
H	-2.222815	-2.194345	2.940663
H	3.146065	-0.755020	3.338724
H	1.560423	-0.664896	2.544011
H	2.254983	-2.231208	2.948842
H	7.187872	-1.403538	-0.956520
H	6.872779	0.259548	-0.456096
H	7.214951	-0.971821	0.762926
H	1.594468	-1.360824	-2.652293
H	3.034697	-2.205118	-3.262874
H	1.840678	-3.067825	-2.276780
H	0.123529	2.932602	3.474737
H	-0.687232	1.392724	3.191998
H	1.077830	1.492765	3.120688
H	2.913868	3.605325	1.406716
H	2.854819	1.862664	1.705640
H	3.296917	2.463051	0.111157
H	1.700281	4.724000	-1.682498
H	2.468041	3.147492	-1.927251
H	0.992609	3.550530	-2.803651
H	-1.905954	4.674453	-1.504258
H	-1.289788	3.514771	-2.691559
H	-2.658927	3.080383	-1.669321
H	-2.781187	3.531693	1.680600
H	-3.263819	2.357933	0.447637
H	-2.640068	1.798374	1.996987

Molecular representation of the optimised geometry of [CpRu*H₃(IMes)] 1** (all hydrogen atoms except those directly attached to the metal are omitted for clarity)



Coordinates of the optimised geometry of [CpRu*H₃(PPy₃)] 3**

(atom, x-, y-, z-positions in Å)

Ru	1.119238	-0.142014	-0.709919
P	-1.068775	-0.020179	-0.220064
N	-1.833984	1.538719	-0.120227
N	-2.193860	-0.843796	-1.254099
N	-1.568648	-0.694865	1.314452
C	-3.188713	1.845705	-0.259502
C	-1.162104	2.703789	0.242840
C	-2.074055	3.722518	0.335017
C	-3.357431	3.178584	0.013848
C	-3.398117	-1.454039	-0.894760
C	-4.023551	-1.873586	-2.040650
C	-3.193356	-1.510729	-3.146829
C	-2.083206	-0.884871	-2.642607
C	3.292084	0.517405	-0.723718
C	3.237698	-0.873791	-0.369892
C	2.579587	-0.979433	0.911409
C	2.244664	0.343294	1.347594
C	2.674671	1.270150	0.342217
C	3.904522	-1.998611	-1.111986
C	2.453097	-2.229227	1.736871
C	1.622694	0.686781	2.672677
C	2.686868	2.769619	0.458329
C	4.024109	1.105153	-1.898434
C	-1.209035	-1.972365	1.734656
C	-1.768307	-2.198006	2.968022
C	-2.495195	-1.021866	3.329402
C	-2.362725	-0.118256	2.304444
H	1.006607	-0.520670	-2.248099
H	0.621054	-1.626281	-1.038789
H	0.667002	1.034106	-1.698118
H	1.563938	-2.206078	2.372827
H	3.326692	-2.347057	2.393990
H	2.393003	-3.123127	1.109237
H	3.936044	-1.805549	-2.187779
H	4.939407	-2.131896	-0.766496
H	3.379978	-2.946410	-0.962974
H	1.121470	1.658195	2.646432
H	2.387877	0.733832	3.460219
H	0.881557	-0.058881	2.976310
H	2.499136	3.255768	-0.503306
H	3.664993	3.118593	0.818770
H	1.938916	3.131777	1.169723
H	3.565734	2.041199	-2.229782
H	5.070069	1.320388	-1.637281
H	4.029846	0.420986	-2.751298
H	-0.605002	-2.603078	1.100024
H	-1.673054	-3.106922	3.547257
H	-3.049267	-0.856674	4.243959

H	-2.750540	0.881488	2.187168
H	-3.677616	-1.551018	0.142944
H	-4.967144	-2.401532	-2.083320
H	-3.387040	-1.702307	-4.193811
H	-1.214355	-0.470379	-3.129757
H	-0.092479	2.688391	0.373197
H	-1.849168	4.750784	0.585318
H	-4.296068	3.715069	-0.032253
H	-3.896188	1.088883	-0.561500

Molecular representation of the optimised geometry of [CpRu*H₃(PPy₃)] **3** (all hydrogen atoms except those directly attached to the metal are omitted for clarity)**

