Electronic Supplementary Information

A diphosphine-carbonyl complex of ruthenium: An efficient precursor for new complexes and C-C and C-N bond coupling catalysis

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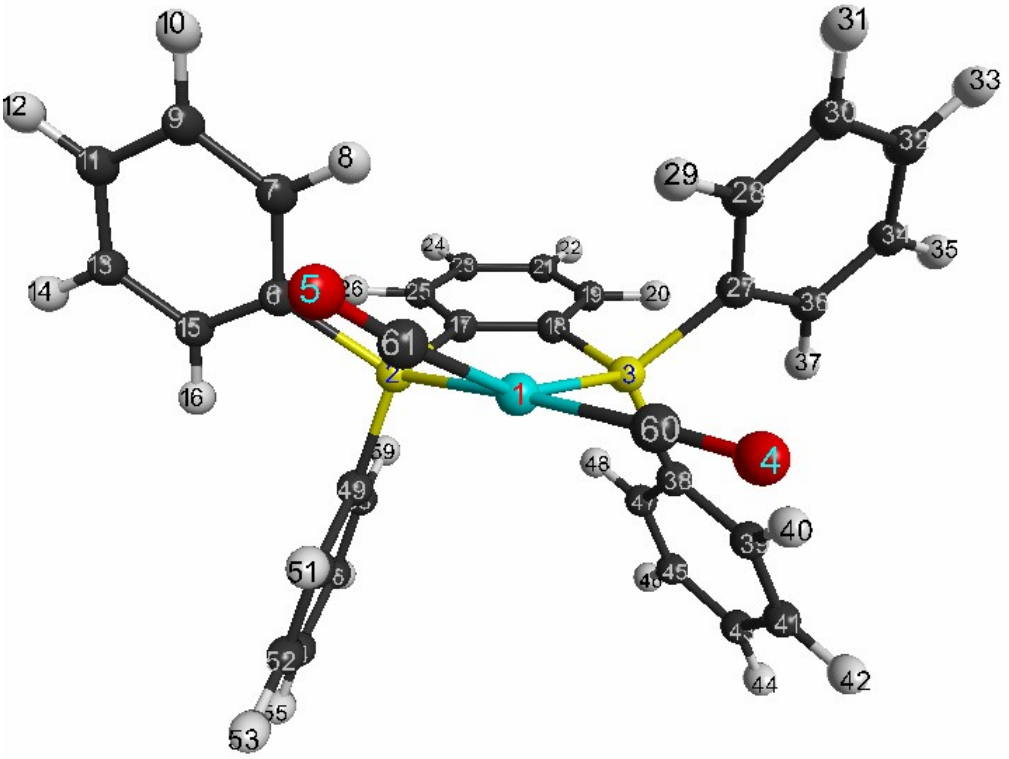
Cartesian coordinates for all molecules in Figs. 9 and 10 with computed electronic and zero-point energies (19 pages).

o-Bz(Ph_2P)$_2$Ru(CO)$_2$ [**1**] ^{1}A RB3LYP/6-31+G(d′)/SDD[Ru] C_1 Geometry	
Nuclear repulsion energy	4559.663270 Hartrees
RB3LYP/6-31+G(d′)/SDD[Ru] energy	-2162.040249 Hartrees
Zero-point energy correction	0.464385 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-2162.222963 Hartrees

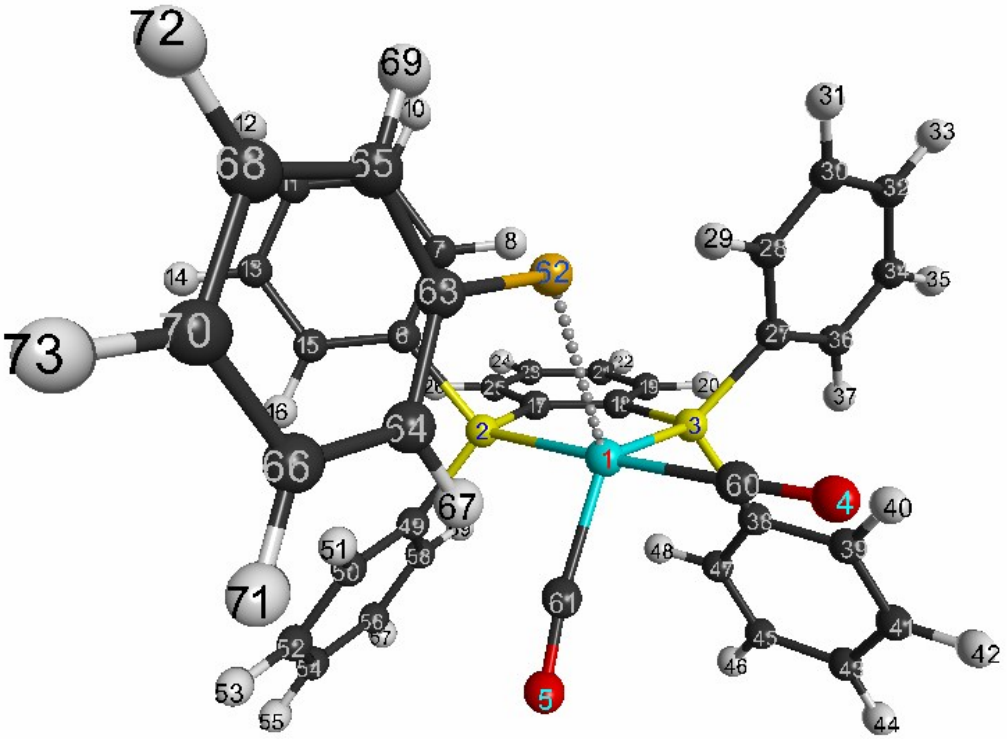


	X	Y	Z		X	Y	Z
Ru1	0.004962	-0.704544	-1.566835	C32	4.975786	-3.087676	1.037350
P2	-1.606514	-0.026350	0.073508	H33	5.765110	-3.807974	1.245276
P3	1.542520	-0.067063	0.138294	C34	5.181361	-1.728156	1.295571
O4	2.212781	-1.246026	-3.593796	H35	6.130863	-1.386017	1.703950
O5	-1.895407	-2.581104	-3.021064	C36	4.170300	-0.800050	1.023644
C6	-3.146204	-0.990864	0.401808	H37	4.348379	0.255845	1.215640
C7	-3.043416	-2.392238	0.453879	C38	2.377006	1.582614	0.000536
H8	-2.080276	-2.868963	0.279437	C39	3.225905	1.793610	-1.103305
C9	-4.170757	-3.175687	0.710329	H40	3.411487	0.986699	-1.810087
H10	-4.077017	-4.259482	0.744278	C41	3.836359	3.032813	-1.305425
C11	-5.418242	-2.570188	0.903679	H42	4.493127	3.175189	-2.161695
H12	-6.298616	-3.181794	1.092666	C43	3.596345	4.089429	-0.417776
C13	-5.531255	-1.178256	0.840095	H44	4.066778	5.057520	-0.579611
H14	-6.499506	-0.700588	0.979815	C45	2.744262	3.894568	0.672104
C15	-4.400735	-0.390280	0.592506	H46	2.546213	4.710708	1.364957
H16	-4.503014	0.691036	0.539796	C47	2.138596	2.649063	0.881541
C17	-0.775988	0.016158	1.732708	H48	1.478837	2.517248	1.735270
C18	0.634068	0.010128	1.759646	C49	-2.195265	1.701523	-0.215550
C19	1.298858	0.015924	2.996115	C50	-2.529533	2.054715	-1.536515
H20	2.385832	-0.008209	3.026475	H51	-2.423455	1.319694	-2.332189
C21	0.577928	0.023826	4.193468	C52	-2.979549	3.343919	-1.833606
H22	1.107714	0.016394	5.144289	H53	-3.233980	3.601686	-2.859963
C23	-0.820582	0.021043	4.165880	C54	-3.088835	4.301777	-0.819015
H24	-1.387696	0.011256	5.094909	H55	-3.432048	5.308153	-1.051968
C25	-1.492620	0.014747	2.940401	C56	-2.746530	3.963338	0.493937

H26	-2.580236	-0.012699	2.923753	H57	-2.821641	4.704986	1.287439
C27	2.942634	-1.224165	0.487572	C58	-2.302690	2.670610	0.795332
C28	2.748569	-2.589682	0.219508	H59	-2.035772	2.425114	1.820379
H29	1.808033	-2.912157	-0.224821	C60	1.368518	-1.069156	-2.817156
C30	3.757614	-3.516003	0.498296	C61	-1.192235	-1.809922	-2.510399
H31	3.595424	-4.570363	0.281662				

o-Bz(Ph_2P)$_2$Ru(CO)$_2$--BrPh [**1′**] ^{1}A RB3LYP/6-31+G(d′)/SDD[Ru] C_1 Geometry

Nuclear repulsion energy	6872.013812 Hartrees
RB3LYP/6-31+G(d′)/SDD[Ru] energy	-4965.098532 Hartrees
Zero-point energy correction	0.555684 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-4965.322633 Hartrees



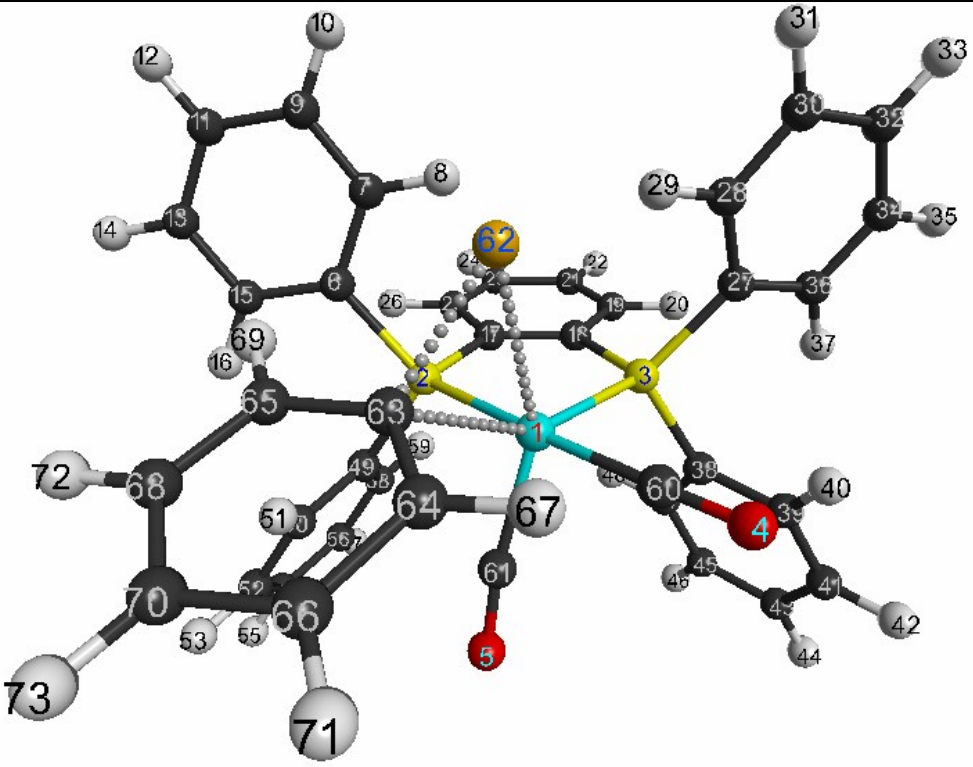
	X	Y	Z		X	Y	Z
Ru1	-0.075584	-0.527405	-0.930211	C38	3.395488	-0.173674	-1.200412
P2	-0.442384	1.449083	0.402528	C39	3.854352	-1.237765	-1.998537
P3	2.040651	-0.478951	0.030471	H40	3.476769	-2.245390	-1.835930
O4	0.649320	-3.043219	-2.502434	C41	4.793460	-1.019083	-3.009333
O5	-0.468669	0.955912	-3.561648	H42	5.134505	-1.856531	-3.615573
C6	-1.709650	1.436815	1.764064	C43	5.288404	0.268957	-3.245389
C7	-1.524770	0.524114	2.819208	H44	6.017725	0.439810	-4.035085
H8	-0.658061	-0.133858	2.821346	C45	4.833267	1.334482	-2.463611
C9	-2.437124	0.455482	3.873513	H46	5.205616	2.342080	-2.641312
H10	-2.272474	-0.254819	4.681896	C47	3.892755	1.115360	-1.450707
C11	-3.558089	1.294115	3.889270	H48	3.545415	1.959156	-0.859237
H12	-4.271381	1.239931	4.709728	C49	-0.794522	3.018753	-0.516799
C13	-3.752934	2.201990	2.845635	C50	-1.938432	3.055589	-1.335815
H14	-4.618023	2.862927	2.848726	H51	-2.583987	2.182022	-1.404188
C15	-2.833797	2.275885	1.791115	C52	-2.246274	4.192254	-2.086084
H16	-2.997767	2.999991	0.998344	H53	-3.136325	4.197832	-2.712510
C17	1.091909	1.799938	1.385893	C54	-1.402090	5.307792	-2.050352
C18	2.202851	0.957350	1.210016	H55	-1.634481	6.189954	-2.643981

C19	3.364100	1.187462	1.968092	C56	-0.250031	5.273613	-1.260906
H20	4.229325	0.541401	1.844583	H57	0.423276	6.128803	-1.237636
C21	3.417369	2.230413	2.894172	C58	0.051002	4.139252	-0.497310
H22	4.322638	2.391137	3.477017	H59	0.955927	4.134712	0.103158
C23	2.301418	3.055030	3.083691	C60	0.372234	-2.082318	-1.917571
H24	2.329906	3.858199	3.817804	C61	-0.413293	0.399737	-2.540161
C25	1.144924	2.837402	2.333979	Br62	-1.932788	-2.014800	0.424133
H26	0.272393	3.467538	2.494610	C63	-3.650532	-2.077364	-0.475232
C27	2.761954	-1.876571	1.041209	C64	-3.783517	-1.500521	-1.733885
C28	1.870336	-2.729094	1.710638	C65	-4.711473	-2.720248	0.163195
H29	0.799608	-2.580263	1.583806	C66	-5.026954	-1.567623	-2.373931
C30	2.337962	-3.771079	2.518029	H67	-2.929484	-1.008991	-2.197473
H31	1.627593	-4.421236	3.025906	C68	-5.948835	-2.777582	-0.488691
C32	3.712649	-3.985573	2.657055	H69	-4.580057	-3.164800	1.146580
H33	4.080382	-4.801681	3.276558	C70	-6.108950	-2.203110	-1.754960
C34	4.613339	-3.153959	1.982040	H71	-5.142921	-1.122738	-3.360655
H35	5.685500	-3.320744	2.073757	H72	-6.786369	-3.274083	-0.001910
C36	4.142343	-2.108924	1.180855	H73	-7.072750	-2.253309	-2.257659
H37	4.857857	-1.484664	0.650520				

o-Bz(Ph_2P)$_2$Ru(CO)$_2$ + PhBr → o-Bz(Ph_2P)$_2$Ru(CO)$_2$(Ph)(Br) [**$TS_{1'\rightarrow 2}$**]

^{1}A RB3LYP/6-31+G(d')/SDD[Ru] C_1 Transition Structure

Nuclear repulsion energy	6988.946659 Hartrees
RB3LYP/6-31+G(d')/SDD[Ru] energy	-4965.066329 Hartrees
Zero-point energy correction	0.554704 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-4965.297412 Hartrees

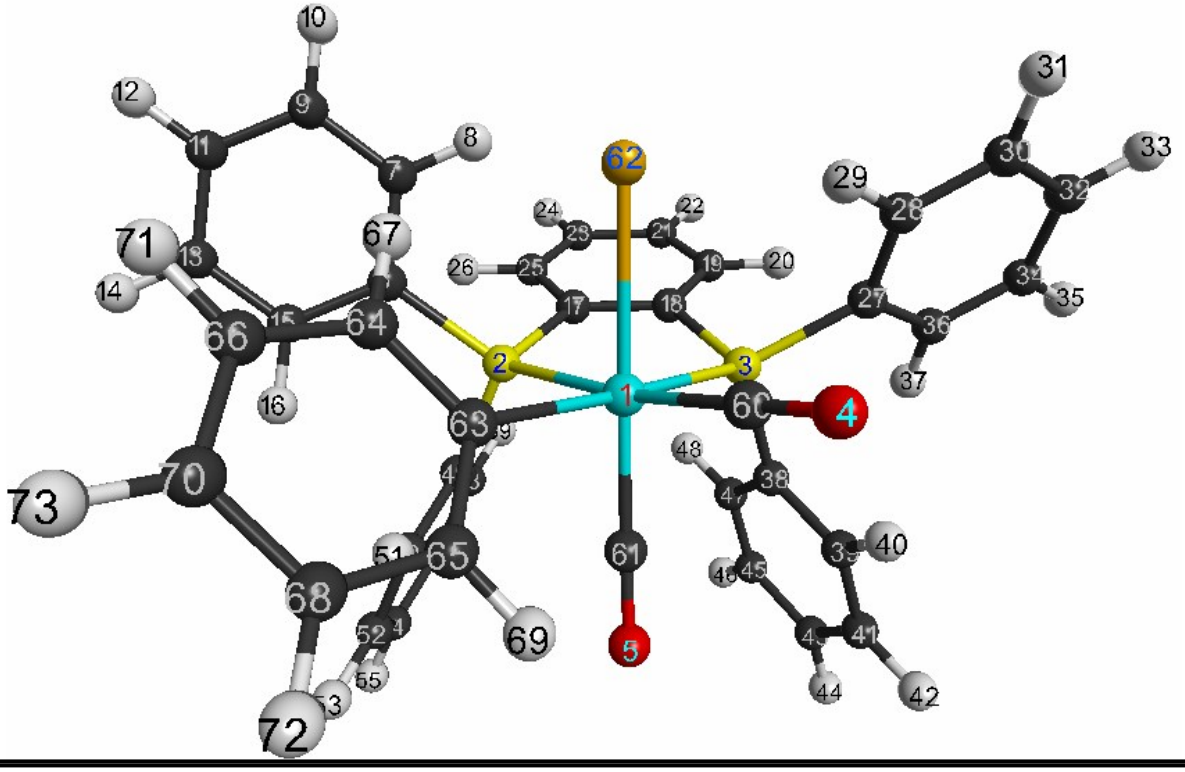


	X	Y	Z		X	Y	Z
Ru1	-0.031081	-0.774835	-0.789255	C38	3.112401	0.749863	-1.197080
P2	-1.027375	1.113944	0.398659	C39	3.867275	-0.152440	-1.969914
P3	1.992146	0.092683	0.121583	H40	3.848252	-1.216530	-1.743226
O4	1.538256	-2.942536	-2.249840	C41	4.647698	0.300914	-3.035802

O5	-0.563387	0.489852	-3.498318	H42	5.225018	-0.413492	-3.619950
C6	-2.260082	0.881043	1.768528	C43	4.681219	1.663431	-3.355956
C7	-1.878571	0.092816	2.869627	H44	5.285566	2.015561	-4.189794
H8	-0.892658	-0.364541	2.894777	C45	3.926640	2.566077	-2.602047
C9	-2.754407	-0.109517	3.938034	H46	3.938163	3.627051	-2.845788
H10	-2.441131	-0.722758	4.780871	C47	3.147375	2.113184	-1.531192
C11	-4.030778	0.465002	3.920475	H48	2.563566	2.831269	-0.960642
H12	-4.715603	0.302114	4.750608	C49	-1.811451	2.395626	-0.682478
C13	-4.420176	1.247692	2.830315	C50	-2.864469	1.981903	-1.520247
H14	-5.408934	1.702641	2.807449	H51	-3.189844	0.943302	-1.513189
C15	-3.540103	1.457781	1.761356	C52	-3.485929	2.886995	-2.382966
H16	-3.858110	2.076376	0.926737	H53	-4.297009	2.546253	-3.023644
C17	0.311573	2.011715	1.319667	C54	-3.051794	4.216332	-2.440504
C18	1.642052	1.579621	1.182089	H55	-3.528042	4.918801	-3.121933
C19	2.657061	2.237167	1.899913	C56	-1.992432	4.631199	-1.629725
H20	3.687765	1.903690	1.806697	H57	-1.636198	5.658811	-1.677231
C21	2.355348	3.303489	2.747584	C58	-1.377597	3.728611	-0.753290
H22	3.151682	3.797825	3.301102	H59	-0.552296	4.072420	-0.136618
C23	1.027120	3.721597	2.897946	C60	0.932039	-2.122233	-1.702978
H24	0.781839	4.540356	3.571855	C61	-0.457213	0.003193	-2.449265
C25	0.012923	3.076203	2.190018	Br62	-0.964292	-2.785827	0.915372
H26	-1.020010	3.390211	2.325157	C63	-2.152971	-2.367058	-0.790354
C27	3.153795	-0.870823	1.206757	C64	-2.071982	-3.315653	-1.825211
C28	2.580078	-1.823039	2.067282	C65	-3.375339	-1.732520	-0.512868
H29	1.506310	-1.994175	2.037930	C66	-3.167885	-3.502903	-2.668501
C30	3.377065	-2.566842	2.942853	H67	-1.157161	-3.876559	-1.990340
H31	2.914985	-3.301560	3.599819	C68	-4.462733	-1.937182	-1.366846
C32	4.762978	-2.378567	2.961657	H69	-3.475190	-1.083885	0.351117
H33	5.385827	-2.962736	3.636730	C70	-4.367421	-2.807581	-2.459881
C34	5.346403	-1.443761	2.099232	H71	-3.080560	-4.208435	-3.493683
H35	6.425304	-1.296739	2.101510	H72	-5.398464	-1.418588	-1.159535
C36	4.548818	-0.694102	1.228306	H73	-5.219615	-2.966210	-3.116878
H37	5.019885	0.022456	0.559573				

o-Bz(Ph_2P)$_2$Ru(CO)$_2$(Ph)(Br) [**2**] ^{1}A RB3LYP/6-31+G(d′)/SDD[Ru] C_1 Geometry

Nuclear repulsion energy	7063.424501 Hartrees
RB3LYP/6-31+G(d′)/SDD[Ru] energy	-4965.157642 Hartrees
Zero-point energy correction	0.557591 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-4965.391202 Hartrees



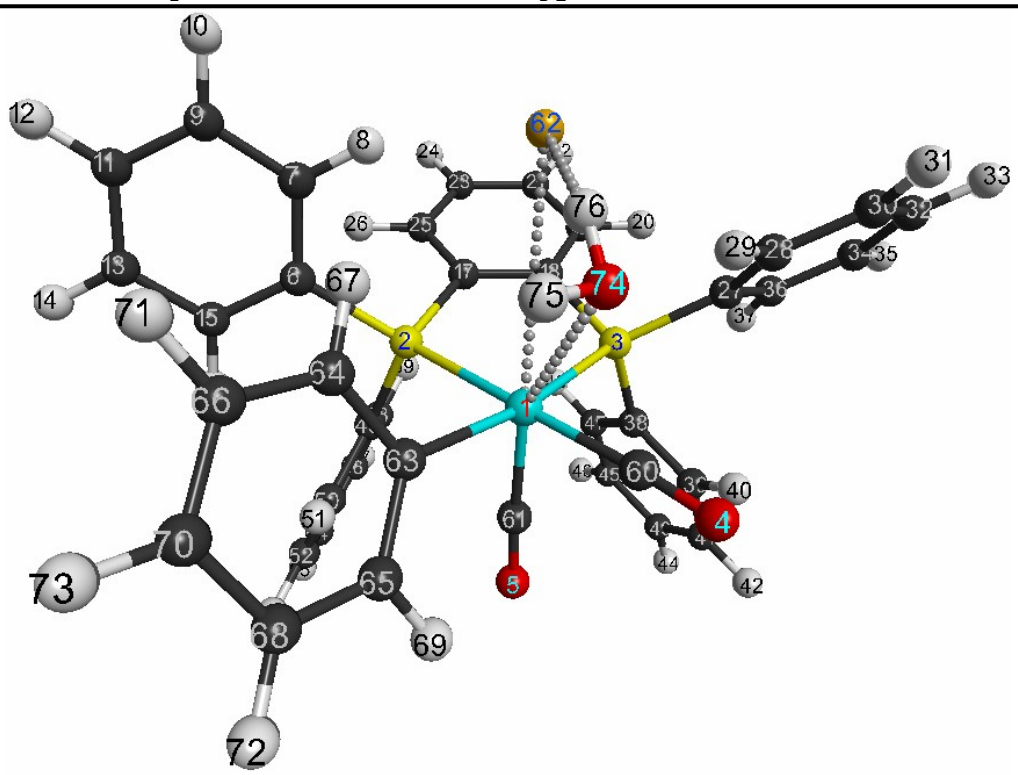
	X	Y	Z		X	Y	Z
Ru1	-0.128386	-0.992816	-0.677544	C38	2.596254	1.332671	-1.200507
P2	-1.176776	0.903035	0.499473	C39	3.150775	0.790844	-2.375348
P3	1.930013	0.156615	0.066587	H40	3.208002	-0.289152	-2.503320
O4	1.127420	-3.537916	-1.820905	C41	3.636391	1.623516	-3.384495
O5	-0.069210	0.367382	-3.371558	H42	4.062827	1.185436	-4.284897
C6	-2.637253	0.672972	1.612634	C43	3.566603	3.014978	-3.242337
C7	-2.468694	0.063855	2.870365	H44	3.939760	3.664705	-4.031641
H8	-1.484353	-0.260109	3.192292	C45	3.010523	3.562901	-2.084230
C9	-3.567095	-0.138096	3.710006	H46	2.948477	4.643093	-1.964715
H10	-3.417830	-0.612065	4.678344	C47	2.529542	2.727659	-1.067803
C11	-4.847744	0.254973	3.306787	H48	2.105894	3.173026	-0.171755
H12	-5.702035	0.092855	3.961646	C49	-1.696499	2.297705	-0.598884
C13	-5.023140	0.856962	2.057794	C50	-2.476610	1.987099	-1.728268
H14	-6.014255	1.166494	1.731411	H51	-2.738530	0.952590	-1.942420
C15	-3.926273	1.064229	1.215178	C52	-2.920023	2.998528	-2.584835
H16	-4.087006	1.534988	0.250140	H53	-3.522920	2.738920	-3.452823
C17	0.101874	1.615908	1.639345	C54	-2.579817	4.331992	-2.334427
C18	1.458250	1.261672	1.477390	H55	-2.918368	5.118555	-3.006236
C19	2.414267	1.760611	2.376192	C56	-1.796762	4.648502	-1.220207
H20	3.456730	1.470548	2.271488	H57	-1.522566	5.682867	-1.019975
C21	2.039663	2.612519	3.417709	C58	-1.359752	3.639108	-0.355588
H22	2.792149	2.981517	4.112118	H59	-0.753310	3.905734	0.505684
C23	0.698944	2.978973	3.569294	C60	0.665573	-2.578200	-1.395351
H24	0.396795	3.638294	4.380773	C61	-0.102564	-0.129075	-2.330252
C25	-0.261524	2.480332	2.686499	Br62	-0.152805	-2.268713	1.631032

H26	-1.306464	2.745673	2.828362	C63	-2.042804	-1.856627	-1.219925
C27	3.472069	-0.712028	0.614982	C64	-3.006220	-2.207844	-0.254862
C28	3.392117	-1.994973	1.183103	C65	-2.379346	-2.121625	-2.565125
H29	2.423595	-2.468417	1.316523	C66	-4.237827	-2.774283	-0.611335
C30	4.552400	-2.657008	1.598156	H67	-2.798274	-2.059273	0.799867
H31	4.470925	-3.650996	2.033953	C68	-3.607586	-2.691126	-2.930269
C32	5.804124	-2.051977	1.452172	H69	-1.675787	-1.896943	-3.365863
H33	6.705260	-2.572143	1.772257	C70	-4.550262	-3.018465	-1.951983
C34	5.893323	-0.775554	0.886182	H71	-4.951602	-3.029943	0.171828
H35	6.862970	-0.296280	0.762567	H72	-3.818078	-2.882149	-3.982594
C36	4.737019	-0.110338	0.468106	H73	-5.505307	-3.463153	-2.228007
H37	4.827637	0.873712	0.015327				

o-Bz(Ph_2P)$_2$Ru(CO)$_2$(Ph)(Br) + H_2O → o-Bz(Ph_2P)$_2$Ru(CO)$_2$(Ph)(OH)-HBr [**$TS_{2\rightarrow 3'}$**]

^{1}A RB3LYP/6-31+G(d')/SDD[Ru] C_1 Transition Structure

Nuclear repulsion energy	7388.639352 Hartrees
RB3LYP/6-31+G(d')/SDD[Ru] energy	-5041.549646 Hartrees
Zero-point energy correction	0.581757 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-5041.818158 Hartrees

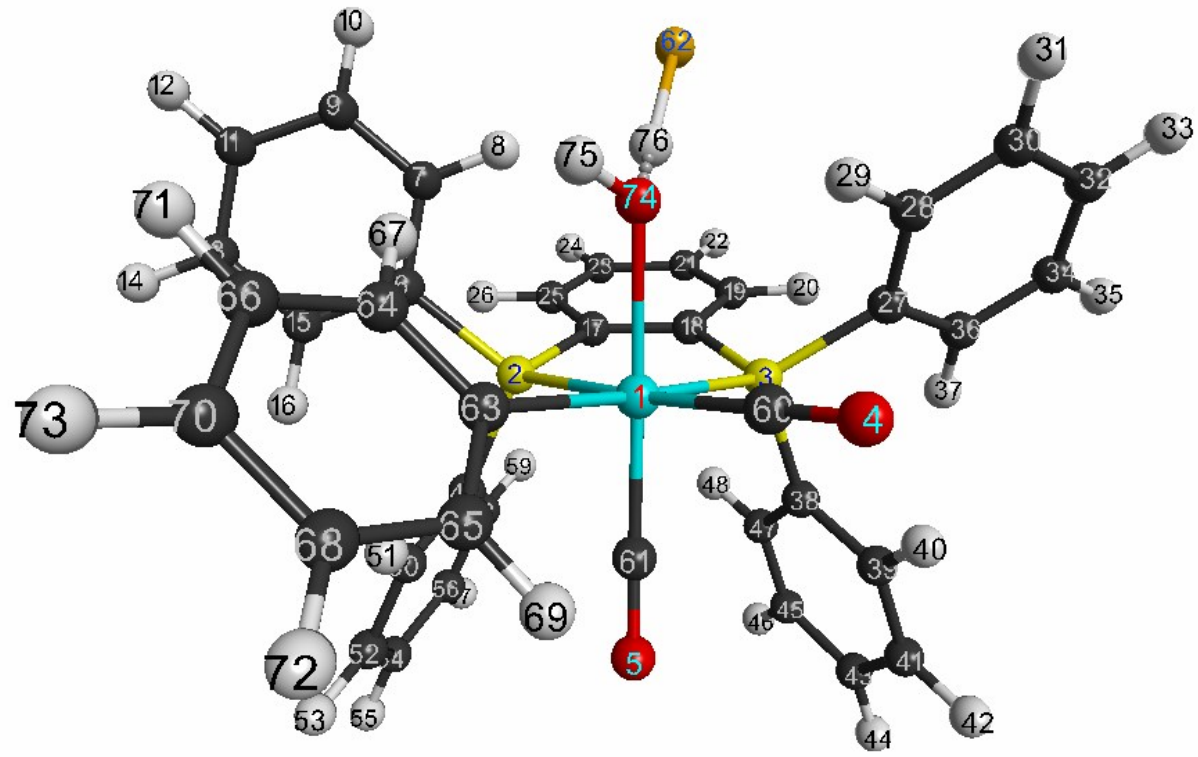


	X	Y	Z		X	Y	Z
Ru1	-0.109211	-0.810960	-0.968800	C39	3.355479	1.059943	-2.072401
P2	-1.204300	0.825058	0.569890	H40	3.438945	0.008819	-2.344575
P3	1.918232	0.090713	0.136421	C41	3.923387	2.025816	-2.904370
O4	1.306579	-2.714175	-2.917145	H42	4.433585	1.718576	-3.815363
O5	0.018085	1.153198	-3.198888	C43	3.834094	3.382885	-2.569804
C6	-2.765684	0.499784	1.521717	H44	4.274445	4.136650	-3.219667
C7	-2.748808	-0.388072	2.613084	C45	3.175702	3.761831	-1.397998
H8	-1.827042	-0.892918	2.891986	H46	3.100325	4.813672	-1.127972
C9	-3.919564	-0.643526	3.332321	C47	2.608978	2.792540	-0.560279
H10	-3.883195	-1.333272	4.173652	H48	2.106967	3.106421	0.350684
C11	-5.123060	-0.027418	2.973942	C49	-1.608641	2.397714	-0.325523

H12	-6.033447	-0.231271	3.535073	C50	-2.398357	2.324260	-1.488374
C13	-5.147450	0.853131	1.889131	H51	-2.738055	1.358033	-1.856816
H14	-6.075589	1.341824	1.598218	C52	-2.755823	3.483480	-2.181393
C15	-3.978275	1.117542	1.168023	H53	-3.367562	3.404804	-3.078043
H16	-4.026312	1.813553	0.337373	C54	-2.320663	4.734503	-1.731188
C17	0.037576	1.314208	1.849831	H55	-2.593225	5.637156	-2.274734
C18	1.396285	0.972078	1.679867	C56	-1.529645	4.817448	-0.581953
C19	2.317906	1.305357	2.681706	H57	-1.183292	5.785618	-0.224540
H20	3.360138	1.017187	2.577423	C58	-1.178060	3.658128	0.118653
C21	1.906481	1.970871	3.839148	H59	-0.567754	3.744640	1.013123
H22	2.633261	2.202420	4.615361	C60	0.781485	-2.044486	-2.151299
C23	0.563510	2.318490	4.003725	C61	-0.048637	0.427126	-2.303928
H24	0.232591	2.827880	4.906628	Br62	0.283473	-2.184735	2.438014
C25	-0.364369	1.989479	3.012576	C63	-2.001221	-1.532226	-1.642539
H26	-1.413345	2.237175	3.156993	C64	-2.842437	-2.158936	-0.699840
C27	3.390682	-0.952318	0.522649	C65	-2.453359	-1.497667	-2.976672
C28	3.271995	-2.350266	0.560199	C66	-4.067607	-2.730529	-1.071793
H29	2.309506	-2.822080	0.399700	H67	-2.550709	-2.205207	0.348724
C30	4.393562	-3.146157	0.815000	C68	-3.681442	-2.059536	-3.353707
H31	4.283183	-4.228244	0.840870	H69	-1.843366	-1.036613	-3.753101
C32	5.640792	-2.557846	1.040663	C70	-4.495621	-2.681630	-2.402383
H33	6.510736	-3.180353	1.242407	H71	-4.688220	-3.205701	-0.312700
C34	5.770333	-1.164931	0.995506	H72	-3.993812	-2.016221	-4.396824
H35	6.740181	-0.697668	1.156889	H73	-5.447813	-3.122181	-2.692999
C36	4.654750	-0.367252	0.729116	O74	-0.008946	-3.560421	-0.311842
H37	4.779063	0.711128	0.660865	H75	-0.897368	-3.874667	-0.533606
C38	2.694356	1.430879	-0.886122	H76	0.011066	-3.392465	0.664778

o-Bz(Ph_2P)$_2$Ru(CO)$_2$(Ph)(OH)-HBr [**3'**] ^{1}A RB3LYP/6-31+G(d')/SDD[Ru] C_1 Geometry

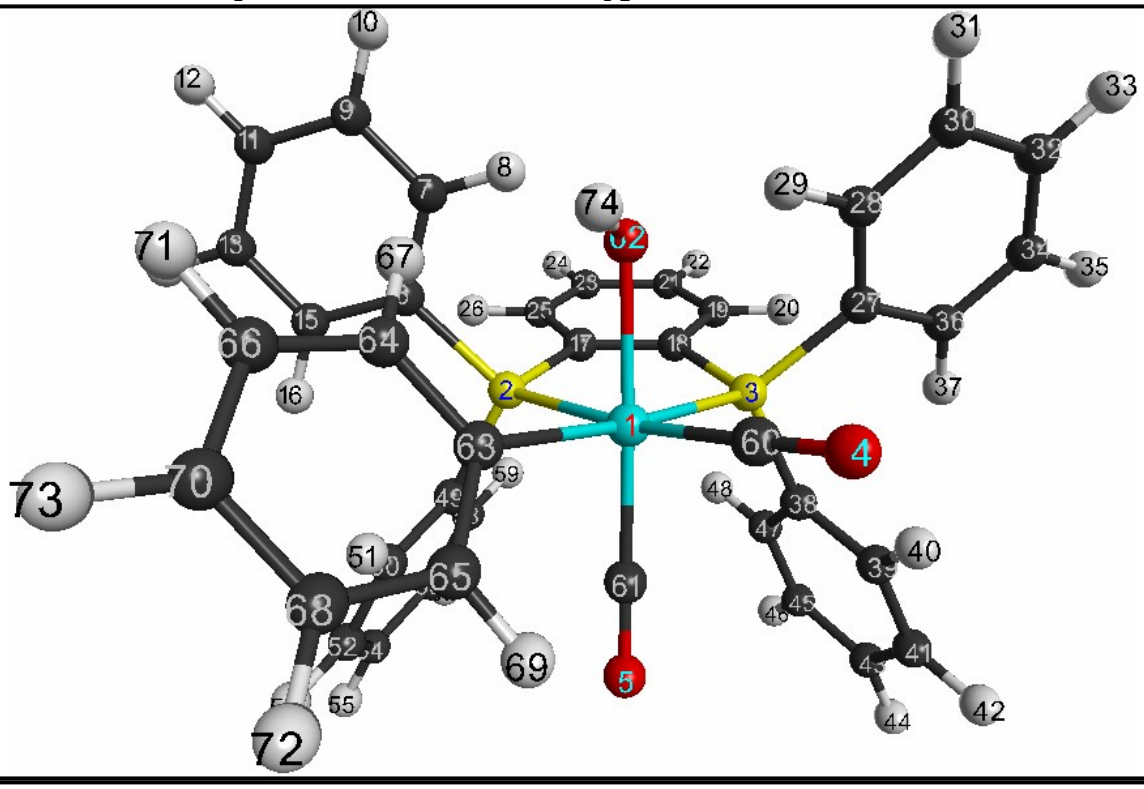
Nuclear repulsion energy	7302.724712 Hartrees
RB3LYP/6-31+G(d')/SDD[Ru] energy	-5041.575491 Hartrees
Zero-point energy correction	0.582082 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-5041.836407 Hartrees



	X	Y	Z		X	Y	Z
Ru1	-0.171663	-0.727979	-1.080354	C39	3.306463	1.108628	-2.230527
P2	-1.231129	0.914190	0.452018	H40	3.347146	0.061612	-2.527138
P3	1.878227	0.152494	-0.013366	C41	3.891792	2.073382	-3.051911
O4	1.247416	-2.811565	-2.822299	H42	4.374878	1.769751	-3.978676
O5	-0.045458	1.239938	-3.355350	C43	3.853739	3.424850	-2.686534
C6	-2.706884	0.461565	1.467315	H44	4.306860	4.177559	-3.328716
C7	-2.548465	-0.461105	2.517774	C45	3.229618	3.800499	-1.494838
H8	-1.572739	-0.881125	2.763419	H46	3.194508	4.848167	-1.201704
C9	-3.652947	-0.848643	3.281631	C47	2.646724	2.832800	-0.666821
H10	-3.507685	-1.561468	4.090989	H48	2.172340	3.142073	0.260621
C11	-4.922013	-0.326027	3.009238	C49	-1.724335	2.486068	-0.381883
H12	-5.779905	-0.630354	3.606344	C50	-2.538014	2.403785	-1.527294
C13	-5.082634	0.592584	1.967167	H51	-2.842238	1.431935	-1.911733
H14	-6.064279	1.009055	1.748432	C52	-2.957976	3.563681	-2.183422
C15	-3.982483	0.985214	1.197510	H53	-3.587413	3.481605	-3.067345
H16	-4.129009	1.702520	0.395524	C54	-2.561036	4.820338	-1.713646
C17	0.030196	1.372684	1.724812	H55	-2.882292	5.723248	-2.229411
C18	1.380432	1.007406	1.545843	C56	-1.744160	4.910333	-0.582805
C19	2.313825	1.292953	2.553312	H57	-1.426307	5.883601	-0.213207
H20	3.347322	0.977007	2.438555	C58	-1.329564	3.751072	0.082072
C21	1.919945	1.943791	3.722961	H59	-0.697185	3.839701	0.961198
H22	2.650489	2.136500	4.505880	C60	0.718767	-2.033541	-2.167396
C23	0.584773	2.320063	3.896600	C61	-0.091770	0.513423	-2.462579
H24	0.267594	2.813471	4.813061	Br62	0.513604	-2.347432	3.338603
C25	-0.353689	2.032420	2.904553	C63	-2.044263	-1.457092	-1.857954
H26	-1.397394	2.293966	3.062249	C64	-3.071387	-1.908118	-1.004371
C27	3.292124	-0.950161	0.404819	C65	-2.284025	-1.585867	-3.243989
C28	3.054983	-2.309872	0.663317	C66	-4.260189	-2.466094	-1.499307
H29	2.048137	-2.710553	0.623221	H67	-2.978238	-1.809176	0.075330
C30	4.115209	-3.157814	0.997973	C68	-3.470393	-2.133722	-3.747600
H31	3.912033	-4.205185	1.209654	H69	-1.532287	-1.262021	-3.963336

C32	5.418912	-2.661369	1.072128	C70	-4.468030	-2.581884	-2.875501
H33	6.241924	-3.324492	1.332435	H71	-5.024763	-2.800245	-0.798656
C34	5.664768	-1.308115	0.811161	H72	-3.608078	-2.216027	-4.825437
H35	6.678104	-0.913959	0.863688	H73	-5.389441	-3.013500	-3.262572
C36	4.608828	-0.456209	0.478340	O74	-0.352482	-2.301287	0.422139
H37	4.816303	0.589578	0.264369	H75	-1.138704	-2.858626	0.339830
C38	2.680853	1.476826	-1.024611	H76	-0.064493	-2.288938	1.411293

o-Bz(Ph_2P)$_2$Ru(CO)$_2$(Ph)(OH) [**3**] ^{1}A RB3LYP/6-31+G(d′)/SDD[Ru] C_1 Geometry	
Nuclear repulsion energy	6143.528881 Hartrees
RB3LYP/6-31+G(d′)/SDD[Ru] energy	-2469.527983 Hartrees
Zero-point energy correction	0.569798 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-2469.757848 Hartrees

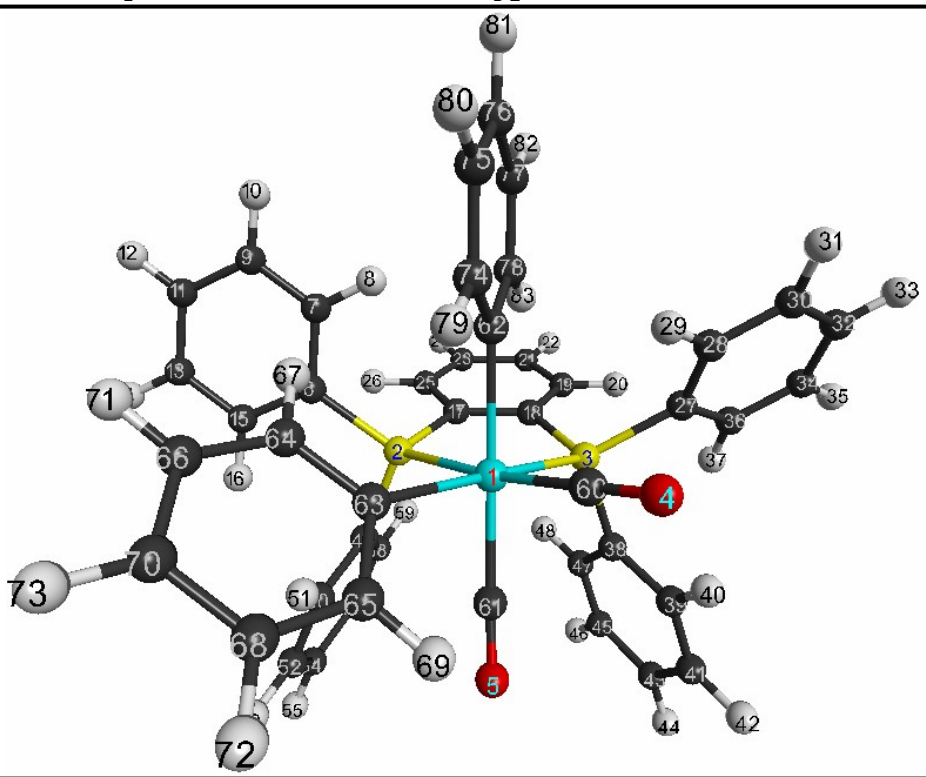


	X	Y	Z		X	Y	Z
Ru1	-0.123560	-1.197486	-0.499232	C38	2.856815	0.753156	-1.227628
P2	-1.187028	0.819620	0.432034	C39	3.444545	-0.095457	-2.184939
P3	1.928502	-0.029002	0.164511	H40	3.385036	-1.176078	-2.064495
O4	1.221216	-3.809188	-1.331177	C41	4.109392	0.432452	-3.292987
O5	-0.084409	-0.120558	-3.340886	H42	4.560283	-0.239739	-4.020591
C6	-2.523283	0.693047	1.699535	C43	4.186168	1.819261	-3.471983
C7	-2.252345	-0.035229	2.874591	H44	4.697908	2.231062	-4.339722
H8	-1.298482	-0.548672	2.972649	C45	3.595717	2.669774	-2.534333
C9	-3.222769	-0.133974	3.874778	H46	3.644398	3.749124	-2.667184
H10	-3.004754	-0.701908	4.777721	C47	2.936105	2.141192	-1.417554
C11	-4.469510	0.483793	3.717054	H48	2.484267	2.818999	-0.698044
H12	-5.223079	0.403149	4.498649	C49	-1.852787	1.997327	-0.822869
C13	-4.743933	1.201018	2.549328	C50	-2.779602	1.488405	-1.752770
H14	-5.711353	1.681759	2.415014	H51	-3.072328	0.440707	-1.710668
C15	-3.775564	1.307109	1.543752	C52	-3.319626	2.316099	-2.740012
H16	-4.004813	1.870267	0.643340	H53	-4.035385	1.906528	-3.450140
C17	0.109747	1.761377	1.369205	C54	-2.930316	3.657820	-2.824396
C18	1.463756	1.386688	1.265678	H55	-3.344616	4.299676	-3.599699
C19	2.430258	2.070552	2.023904	C56	-1.999128	4.166849	-1.914769
H20	3.473143	1.766934	1.967146	H57	-1.683744	5.206869	-1.978442
C21	2.064734	3.121805	2.865411	C58	-1.464606	3.343107	-0.917111
H22	2.824385	3.637576	3.449895	H59	-0.741651	3.756313	-0.218892
C23	0.719749	3.496341	2.967607	C60	0.719750	-2.819906	-1.029333
H24	0.423846	4.305826	3.632298	C61	-0.098533	-0.510835	-2.253668
C25	-0.248902	2.814921	2.229849	O62	-0.192465	-1.890125	1.497197

H26	-1.296096	3.088932	2.337712	C63	-2.010602	-2.165680	-0.893499
C27	3.234409	-0.919135	1.117657	C64	-2.950811	-2.397951	0.130311
C28	2.819301	-1.903375	2.034053	C65	-2.357023	-2.647616	-2.175458
H29	1.752538	-2.121124	2.124869	C66	-4.162508	-3.064254	-0.106488
C30	3.771713	-2.586097	2.797763	H67	-2.750719	-2.048080	1.139505
H31	3.444603	-3.348510	3.502912	C68	-3.564579	-3.314126	-2.422978
C32	5.134406	-2.302541	2.654559	H69	-1.674334	-2.512927	-3.013903
H33	5.871105	-2.841470	3.248137	C70	-4.479375	-3.527094	-1.386557
C34	5.549331	-1.328709	1.739607	H71	-4.859435	-3.215256	0.718121
H35	6.608149	-1.106640	1.617069	H72	-3.784175	-3.670952	-3.429347
C36	4.604621	-0.637721	0.973568	H73	-5.418606	-4.045693	-1.573213
H37	4.941347	0.109631	0.258900	H74	-0.715913	-2.701612	1.524132

o-Bz(Ph_2P)$_2$Ru(CO)$_2$(Ph)$_2$ [**4**] ^{1}A RB3LYP/6-31+G(d')/SDD[Ru] C_1 Geometry

Nuclear repulsion energy	7240.130512 Hartrees
RB3LYP/6-31+G(d')/SDD[Ru] energy	-2625.319079 Hartrees
Zero-point energy correction	0.646646 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-2625.577073 Hartrees



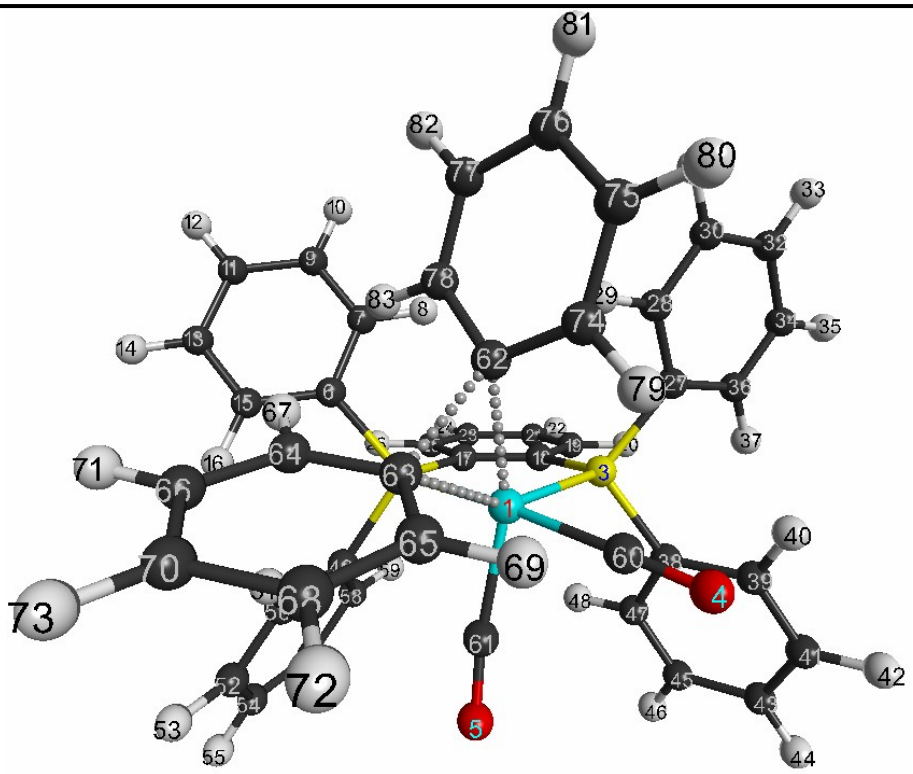
	X	Y	Z		X	Y	Z
Ru1	-0.113697	-0.532984	-1.085426	C43	3.975479	3.863656	-1.684599
P2	-1.137698	0.729777	0.778654	H44	4.440445	4.742755	-2.126663
P3	1.941427	0.060968	0.107577	C45	3.336295	3.953435	-0.446150
O4	1.190298	-2.297931	-3.195824	H46	3.300308	4.903526	0.084015
O5	0.130958	1.929078	-2.918236	C47	2.736748	2.822593	0.123142
C6	-2.661899	0.220400	1.710556	H48	2.247342	2.912060	1.089151
C7	-2.696407	-1.034264	2.347111	C49	-1.513810	2.491612	0.348840
H8	-1.845553	-1.704906	2.280823	C50	-2.315766	2.728733	-0.783371
C9	-3.829212	-1.440286	3.056339	H51	-2.675637	1.892451	-1.379811
H10	-3.834913	-2.417010	3.536594	C52	-2.654845	4.032914	-1.152056
C11	-4.949026	-0.605101	3.139481	H53	-3.276189	4.196523	-2.030390
H12	-5.832730	-0.925181	3.688623	C54	-2.188242	5.120163	-0.404656

C13	-4.925353	0.640742	2.507808	H55	-2.445711	6.136360	-0.697523
H14	-5.789884	1.300079	2.561384	C56	-1.384771	4.894277	0.716550
C15	-3.790638	1.052161	1.798575	H57	-1.013641	5.733585	1.302351
H16	-3.797342	2.024493	1.316170	C58	-1.052677	3.587931	1.094381
C17	0.134859	0.839526	2.130978	H59	-0.432393	3.432587	1.973062
C18	1.484688	0.533130	1.848876	C60	0.698779	-1.628443	-2.398051
C19	2.430169	0.578113	2.886413	C61	0.031178	1.046317	-2.185596
H20	3.466658	0.321036	2.685671	C62	-0.359730	-2.449710	-0.008063
C21	2.053115	0.924766	4.186080	C63	-2.025336	-0.870834	-2.055355
H22	2.798634	0.941918	4.978934	C64	-3.176289	-1.306754	-1.367753
C23	0.718467	1.234477	4.464457	C65	-2.188812	-0.641194	-3.439901
H24	0.413452	1.497370	5.475608	C66	-4.410978	-1.482697	-2.008333
C25	-0.231831	1.189022	3.441938	H67	-3.119287	-1.539716	-0.309032
H26	-1.272804	1.407476	3.668496	C68	-3.415404	-0.822877	-4.094470
C27	3.396125	-1.079725	0.254255	H69	-1.342830	-0.316077	-4.044962
C28	3.231819	-2.455241	0.023994	C70	-4.541582	-1.239916	-3.379108
H29	2.251345	-2.851249	-0.218852	H71	-5.270088	-1.818876	-1.427407
C30	4.323674	-3.326055	0.112689	H72	-3.483654	-0.637740	-5.166578
H31	4.174810	-4.388350	-0.070493	H73	-5.498056	-1.380672	-3.880502
C32	5.593636	-2.835089	0.426581	C74	-0.992569	-3.548371	-0.635323
H33	6.442698	-3.513261	0.491045	C75	-1.137053	-4.797714	-0.017207
C34	5.771876	-1.463807	0.644398	C76	-0.648186	-5.011916	1.275575
H35	6.759834	-1.068792	0.874829	C77	-0.005834	-3.955559	1.926911
C36	4.683634	-0.592266	0.553441	C78	0.136320	-2.713742	1.288896
H37	4.846181	0.473965	0.693586	H79	-1.398823	-3.433690	-1.637414
C38	2.768237	1.588187	-0.541933	H80	-1.633780	-5.605733	-0.554529
C39	3.408454	1.509947	-1.792934	H81	-0.758799	-5.980850	1.760452
H40	3.440601	0.563506	-2.330484	H82	0.394128	-4.091387	2.932371
C41	4.010127	2.635637	-2.357128	H83	0.656649	-1.937172	1.846695
H42	4.501143	2.554844	-3.325104				

o-Bz(Ph2P)$_2$Ru(CO)$_2$(Ph)$_2$ → o-Bz(Ph2P)$_2$Ru(CO)$_2$ + Ph$_2$ [**TS$_{4\rightarrow1}$**]

^{1}A RB3LYP/6-31+G(d')/SDD[Ru] C_1 Transition Structure

Nuclear repulsion energy	7213.117116 Hartrees
RB3LYP/6-31+G(d')/SDD[Ru] energy	-2625.262267 Hartrees
Zero-point energy correction	0.644663 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-2625.517505 Hartrees

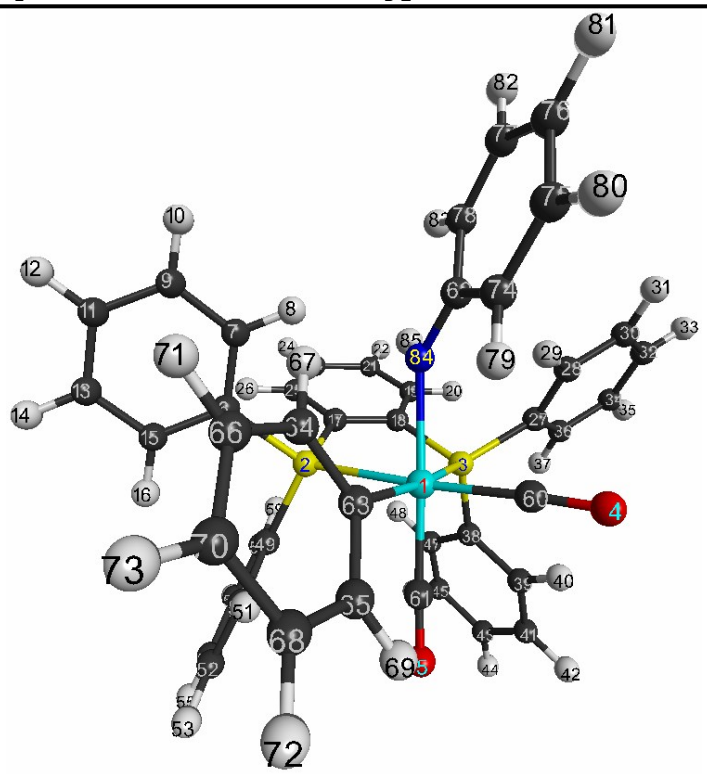


	X	Y	Z		X	Y	Z
Ru1	0.065700	0.453911	-1.063078	C43	-4.535243	-2.825676	-2.846457
P2	1.225287	-0.939872	0.667746	H44	-5.123981	-3.397040	-3.561608
P3	-1.911512	-0.335268	0.103359	C45	-3.579505	-3.464473	-2.050712
O4	-1.819540	1.508450	-3.190593	H46	-3.417163	-4.536847	-2.143927
O5	0.530460	-1.765543	-3.136231	C47	-2.820872	-2.729982	-1.133638
C6	2.349874	-0.366921	2.044037	H48	-2.077098	-3.244613	-0.529938
C7	1.785182	0.304966	3.144936	C49	2.205706	-2.313017	-0.105433
H8	0.710604	0.468655	3.191793	C50	3.206509	-1.955114	-1.029241
C9	2.587998	0.764845	4.191164	H51	3.371901	-0.908192	-1.275753
H10	2.128993	1.277460	5.034657	C52	3.976504	-2.934153	-1.661208
C11	3.973526	0.568594	4.154254	H53	4.743483	-2.634026	-2.372668
H12	4.599721	0.928177	4.968533	C54	3.745677	-4.289327	-1.400881
C13	4.545354	-0.093695	3.065112	H55	4.337433	-5.052706	-1.902554
H14	5.620928	-0.256539	3.025767	C56	2.736789	-4.655588	-0.506566
C15	3.740315	-0.559551	2.018160	H57	2.534144	-5.707038	-0.310180
H16	4.205709	-1.084293	1.188632	C58	1.973428	-3.675706	0.139451
C17	-0.073981	-1.786269	1.688953	H59	1.188252	-3.988634	0.820794
C18	-1.434213	-1.541370	1.435908	C60	-1.078630	1.146924	-2.378142
C19	-2.407356	-2.172953	2.231995	C61	0.421440	-0.979408	-2.294528
H20	-3.461344	-1.984235	2.046471	C62	0.508560	2.613491	-0.361953
C21	-2.039613	-3.030709	3.267564	C63	1.721627	1.893218	-1.554000
H22	-2.806571	-3.508593	3.874335	C64	3.017834	1.689806	-1.002781
C23	-0.683646	-3.259640	3.532947	C65	1.710007	2.452653	-2.865256

H24	-0.385460	-3.913969	4.350004	C66	4.188134	1.977522	-1.705480
C25	0.288859	-2.637123	2.751841	H67	3.119995	1.329457	0.016498
H26	1.340148	-2.800288	2.977469	C68	2.876779	2.736853	-3.569743
C27	-3.111248	0.762919	1.001307	H69	0.762918	2.673082	-3.350847
C28	-2.615683	1.964318	1.533859	C70	4.137341	2.496712	-3.004653
H29	-1.579119	2.243666	1.368252	H71	5.150393	1.800654	-1.224435
C30	-3.450461	2.817100	2.264541	H72	2.798967	3.149684	-4.575168
H31	-3.045960	3.745634	2.662380	H73	5.048968	2.725896	-3.552428
C32	-4.793735	2.486513	2.463370	C74	-0.309795	3.658813	-0.876482
H33	-5.445399	3.153932	3.024698	C75	-0.615820	4.804507	-0.143734
C34	-5.301274	1.297464	1.926032	C76	-0.116470	4.982719	1.153089
H35	-6.348610	1.035431	2.067914	C77	0.707276	3.982141	1.685918
C36	-4.467452	0.442120	1.200334	C78	1.012092	2.839612	0.946801
H37	-4.883305	-0.469818	0.778783	H79	-0.704516	3.593840	-1.886780
C38	-3.009932	-1.344603	-0.992151	H80	-1.250549	5.566691	-0.594861
C39	-3.965698	-0.709771	-1.806593	H81	-0.344807	5.881924	1.721901
H40	-4.123575	0.363631	-1.730254	H82	1.126656	4.092612	2.685990
C41	-4.723302	-1.444807	-2.722562	H83	1.683752	2.118211	1.396358
H42	-5.457595	-0.933786	-3.342654				

o-Bz(Ph_2P)$_2$Ru(NHPh)(Ph)(CO)$_2$ [**4′**] ^{1}A RB3LYP/6-31+G(d′)/SDD[Ru] C_1 Geometry

Nuclear repulsion energy	7461.972489 Hartrees
RB3LYP/6-31+G(d′)/SDD[Ru] energy	-2680.691776 Hartrees
Zero-point energy correction	0.663133 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-2680.958051 Hartrees



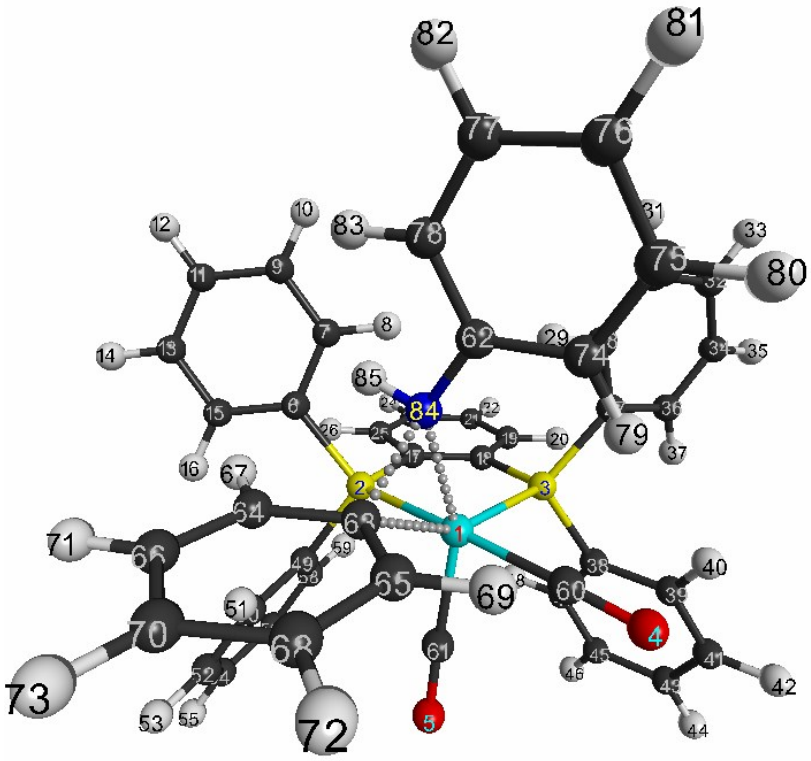
	X	Y	Z		X	Y	Z
Ru1	-0.147315	-0.574542	-0.959810	H44	4.488599	4.699136	-2.208575
P2	-1.151241	0.875495	0.768545	C45	3.458253	3.949700	-0.464253
P3	1.932669	0.120237	0.154791	H46	3.504462	4.895576	0.072562
O4	1.121614	-2.451136	-3.009880	C47	2.842205	2.844525	0.136228
O5	0.077230	1.641075	-3.031496	H48	2.422636	2.947329	1.133418

C6	-2.696632	0.425723	1.682005	C49	-1.456606	2.620530	0.248727
C7	-2.760536	-0.802534	2.366916	C50	-2.233592	2.827855	-0.906335
H8	-1.922435	-1.491057	2.322255	H51	-2.620725	1.976064	-1.462931
C9	-3.909699	-1.158718	3.075819	C52	-2.516665	4.123416	-1.346082
H10	-3.941995	-2.115616	3.593360	H53	-3.119568	4.266200	-2.240682
C11	-5.014455	-0.300121	3.109047	C54	-2.018398	5.228439	-0.646826
H12	-5.910774	-0.581950	3.658613	H55	-2.232832	6.237296	-0.994434
C13	-4.961194	0.918300	2.427637	C56	-1.239816	5.030798	0.497340
H14	-5.814750	1.593601	2.442559	H57	-0.845991	5.884834	1.045653
C15	-3.809687	1.281265	1.719390	C58	-0.962641	3.734397	0.945690
H16	-3.789672	2.234423	1.199825	H59	-0.360444	3.598845	1.840304
C17	0.107253	0.981322	2.133056	C60	0.635726	-1.775909	-2.217378
C18	1.452030	0.629535	1.875438	C61	-0.035552	0.815375	-2.232436
C19	2.385625	0.665010	2.924815	C62	-0.343961	-3.457754	0.592127
H20	3.415855	0.370935	2.739804	C63	-2.097554	-1.102164	-1.736315
C21	2.003473	1.054103	4.210637	C64	-3.032710	-1.805983	-0.955269
H22	2.738612	1.066334	5.013132	C65	-2.505469	-0.762795	-3.044418
C23	0.675607	1.412619	4.463814	C66	-4.306049	-2.135803	-1.438203
H24	0.367107	1.708875	5.464586	H67	-2.761145	-2.121884	0.046236
C25	-0.264260	1.371388	3.431648	C68	-3.776334	-1.091218	-3.538925
H26	-1.301102	1.624458	3.640398	H69	-1.827881	-0.238193	-3.716850
C27	3.343075	-1.054255	0.373569	C70	-4.690089	-1.777131	-2.734086
C28	3.094307	-2.437355	0.361280	H71	-4.994716	-2.683853	-0.795178
H29	2.082429	-2.805436	0.224654	H72	-4.043825	-0.811091	-4.557932
C30	4.144284	-3.346078	0.529405	H73	-5.678112	-2.035569	-3.112329
H31	3.930532	-4.412812	0.516675	C74	-0.760310	-4.213512	-0.534245
C32	5.453080	-2.886730	0.704391	C75	-0.843927	-5.605735	-0.482032
H33	6.269650	-3.595638	0.829256	C76	-0.520471	-6.316441	0.681234
C34	5.711365	-1.511123	0.708370	C77	-0.107159	-5.589619	1.805921
H35	6.728756	-1.144598	0.834053	C78	-0.018427	-4.198585	1.765419
C36	4.664780	-0.599338	0.542556	H79	-1.045720	-3.696697	-1.444774
H37	4.884311	0.465701	0.529452	H80	-1.172975	-6.142627	-1.371509
C38	2.769815	1.616384	-0.538169	H81	-0.588559	-7.401792	0.711103
C39	3.322019	1.518040	-1.829045	H82	0.154055	-6.110240	2.727415
H40	3.271364	0.576346	-2.373537	H83	0.312321	-3.655982	2.653480
C41	3.941556	2.618122	-2.423918	N84	-0.258583	-2.080189	0.591326
H42	4.363718	2.523004	-3.422464	H85	0.152743	-1.777188	1.469231
C43	4.010675	3.839614	-1.742525				

o-Bz(Ph_2P)$_2$Ru(NHPh)(Ph)(CO)$_2$ → o-Bz(Ph_2P)$_2$Ru(CO)$_2$ + Ph_2NH [**$TS_{4'\rightarrow 1}$**]

^{1}A RB3LYP/6-31+G(d')/SDD[Ru] C_1 Transition Structure

Nuclear repulsion energy	7417.908601 Hartrees
RB3LYP/6-31+G(d')/SDD[Ru] energy	-2680.627802 Hartrees
Zero-point energy correction	0.661750 Hartrees
RB3LYP-D3/6-31+G(2d,p)/SDD[Ru] PCM energy (ε=17.2)	-2680.891658 Hartrees



	X	Y	Z		X	Y	Z
Ru1	0.145754	-0.082965	-1.044412	H44	-6.084313	-2.694388	-2.932632
P2	0.787411	-1.429795	0.924895	C45	-4.665831	-2.879077	-1.312315
P3	-2.047448	-0.021428	0.163809	H46	-4.879626	-3.931341	-1.133191
O4	-1.259278	1.178687	-3.435488	C47	-3.708433	-2.227560	-0.527376
O5	-0.215511	-2.647848	-2.645425	H48	-3.192347	-2.785706	0.250169
C6	2.089050	-0.851534	2.115644	C49	1.262102	-3.172975	0.529471
C7	1.880231	0.374394	2.775831	C50	2.281779	-3.365933	-0.422662
H8	0.964169	0.937985	2.605051	H51	2.757221	-2.509114	-0.896672
C9	2.831924	0.873823	3.668526	C52	2.677337	-4.655124	-0.786503
H10	2.652280	1.822356	4.171128	H53	3.466396	-4.782762	-1.524945
C11	4.009393	0.157257	3.913066	C54	2.047904	-5.771265	-0.224388
H12	4.753125	0.547629	4.604948	H55	2.349285	-6.775275	-0.517228
C13	4.223701	-1.061789	3.264106	C56	1.017588	-5.588771	0.701695
H14	5.134570	-1.627895	3.450114	H57	0.508480	-6.449534	1.131692
C15	3.270469	-1.565017	2.370560	C58	0.626894	-4.298566	1.078929
H16	3.452994	-2.514998	1.875278	H59	-0.183544	-4.182570	1.792184
C17	-0.655567	-1.558753	2.086234	C60	-0.666840	0.757204	-2.537305
C18	-1.894434	-0.986968	1.744697	C61	-0.078359	-1.694725	-2.004486
C19	-2.968712	-1.086932	2.648296	C62	1.406615	2.988007	-0.551509
H20	-3.927897	-0.642217	2.395509	C63	2.205430	0.618841	-1.662448
C21	-2.817096	-1.733032	3.874356	C64	3.394802	0.005741	-1.150450
H22	-3.658700	-1.796709	4.561660	C65	2.339556	1.218739	-2.956060
C23	-1.575791	-2.278933	4.224926	C66	4.573098	-0.063576	-1.893204

H24	-1.441567	-2.766448	5.188691	H67	3.402361	-0.399625	-0.141851
C25	-0.504261	-2.187240	3.337825	C68	3.524573	1.136641	-3.682191
H26	0.463168	-2.594285	3.623807	H69	1.500472	1.738490	-3.407815
C27	-2.823235	1.553251	0.757816	C70	4.661142	0.484801	-3.179340
C28	-1.958803	2.620085	1.056913	H71	5.439927	-0.553492	-1.447218
H29	-0.890508	2.514937	0.884084	H72	3.553691	1.591271	-4.672835
C30	-2.461391	3.830382	1.545290	H73	5.579197	0.422895	-3.758631
H31	-1.775474	4.647186	1.760973	C74	0.563188	3.670248	-1.449162
C32	-3.837656	3.993845	1.730615	C75	0.624998	5.061484	-1.568249
H33	-4.231451	4.938283	2.101880	C76	1.517420	5.811817	-0.795599
C34	-4.709162	2.942707	1.421797	C77	2.363185	5.142636	0.100004
H35	-5.783022	3.066225	1.552683	C78	2.316258	3.754123	0.215147
C36	-4.207125	1.730359	0.939269	H79	-0.159608	3.118443	-2.039082
H37	-4.899097	0.928740	0.691397	H80	-0.041483	5.561010	-2.269958
C38	-3.413409	-0.869393	-0.737569	H81	1.557270	6.894907	-0.890588
C39	-4.088702	-0.184665	-1.766559	H82	3.073080	5.704248	0.705721
H40	-3.868398	0.862604	-1.962882	H83	2.995306	3.243816	0.898069
C41	-5.046898	-0.836279	-2.546379	N84	1.412688	1.590473	-0.417393
H42	-5.559162	-0.288074	-3.334922	H85	1.978336	1.346573	0.387568
C43	-5.340803	-2.186404	-2.321526				

Phenylboronic Acid ^{1}A′ RB3LYP/6-31+G(d′) C_s Geometry

Nuclear repulsion energy	392.126020 Hartrees
RB3LYP/6-31+G(d′) energy	-408.270770 Hartrees
Zero-point energy correction	0.124671 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-408.324773 Hartrees

	X	Y	Z		X	Y	Z
C1	1.365293	-1.854526	0.000000	H9	-2.129009	-0.163982	0.000000
C2	1.254484	-0.460947	0.000000	H10	-1.951727	-2.640846	0.000000
C3	0.000000	0.178886	0.000000	H11	0.289945	-3.728794	0.000000
C4	-1.149431	-0.637197	0.000000	B12	-0.153929	1.738315	0.000000
C5	-1.049734	-2.031038	0.000000	O13	-1.412944	2.277737	0.000000
C6	0.209348	-2.642992	0.000000	H14	-1.388131	3.244204	0.000000
H7	2.347652	-2.323685	0.000000	O15	0.897147	2.629444	0.000000
H8	2.175064	0.125798	0.000000	H16	1.772475	2.225169	0.000000

Biphenyl ^{1}A RB3LYP/6-31+G(d′) D_2 Geometry

Nuclear repulsion energy	597.506512 Hartrees
RB3LYP/6-31+G(d′) energy	-463.307454 Hartrees
Zero-point energy correction	0.181188 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-463.352694 Hartrees

	X	Y	Z		X	Y	Z
C1	0.000000	0.000000	0.743742	C12	0.414413	1.133797	-1.467508
C2	-0.414413	1.133797	1.467508	H13	-0.763504	2.013563	0.930186
C3	-0.414295	1.134849	2.865074	H14	-0.747424	2.020971	3.402791
C4	0.000000	0.000000	3.570906	H15	0.000000	0.000000	4.659302
C5	0.414295	-1.134849	2.865074	H16	0.747424	-2.020971	3.402791
C6	0.414413	-1.133797	1.467508	H17	0.763504	-2.013563	0.930186
C7	0.000000	0.000000	-0.743742	H18	-0.763504	-2.013563	-0.930186
C8	-0.414413	-1.133797	-1.467508	H19	-0.747424	-2.020971	-3.402791
C9	-0.414295	-1.134849	-2.865074	H20	0.000000	0.000000	-4.659302
C10	0.000000	0.000000	-3.570906	H21	0.747424	2.020971	-3.402791

C11	0.414295	1.134849	-2.865074	H22	0.763504	2.013563	-0.930186

Aniline ^{1}A′ RB3LYP/6-31+G(d′) C_s Geometry

Nuclear repulsion energy	270.421330 Hartrees
RB3LYP/6-31+G(d′) energy	-287.607024 Hartrees
Zero-point energy correction	0.116904 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-287.642099 Hartrees

	X	Y	Z		X	Y	Z
C1	0.002955	0.940560	0.000000	H8	0.009058	0.763501	2.156111
C2	0.002994	0.222153	1.210200	H9	0.002198	-1.708670	2.154039
C3	0.003140	-1.174429	1.205175	H10	0.002038	-2.974163	0.000000
C4	0.002898	-1.886480	0.000000	H11	0.002198	-1.708670	-2.154039
C5	0.003140	-1.174429	-1.205175	H12	0.009058	0.763501	-2.156111
C6	0.002994	0.222153	-1.210200	H13	-0.274605	2.794298	-0.839124
N7	0.062278	2.340579	0.000000	H14	-0.274605	2.794298	0.839124

Diphenylamine ^{1}A RB3LYP/6-31+G(d′) C_2 Geometry

Nuclear repulsion energy	690.913466 Hartrees
RB3LYP/6-31+G(d′) energy	-518.654756 Hartrees
Zero-point energy correction	0.197512 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-518.709266 Hartrees

	X	Y	Z		X	Y	Z
C1	-0.018860	1.267608	-0.445085	H13	0.000000	0.000000	-2.053177
C2	0.453892	2.368211	-1.187726	C14	0.018860	-1.267608	-0.445085
C3	0.407893	3.658485	-0.658559	C15	0.540607	-1.498122	0.842208
C4	-0.094452	3.882182	0.628732	C16	-0.453892	-2.368211	-1.187726
C5	-0.566528	2.792441	1.368327	C17	0.566528	-2.792441	1.368327
C6	-0.540607	1.498122	0.842208	H18	0.948302	-0.673087	1.418881
N7	0.000000	0.000000	-1.043477	C19	-0.407893	-3.658485	-0.658559
H8	0.864649	2.202860	-2.183615	H20	-0.864649	-2.202860	-2.183615
H9	0.778197	4.491411	-1.253916	C21	0.094452	-3.882182	0.628732
H10	-0.121181	4.886670	1.045156	H22	0.976460	-2.947795	2.365062
H11	-0.976460	2.947795	2.365062	H23	-0.778197	-4.491411	-1.253916
H12	-0.948302	0.673087	1.418881	H24	0.121181	-4.886670	1.045155

PhBr ^{1}A$_1$ RB3LYP/6-31+G(d′) C_{2v} Geometry

Nuclear repulsion energy	429.456182 Hartrees
RB3LYP/6-31+G(d′) energy	-2803.059008 Hartrees
Zero-point energy correction	0.090663 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-2803.082825 Hartrees

	X	Y	Z		X	Y	Z
C1	0.000000	0.000000	-0.097339	Br7	0.000000	0.000000	1.810197
C2	0.000000	1.217087	-0.783059	H8	0.000000	2.154443	-0.233507
C3	0.000000	1.209960	-2.182383	H9	0.000000	2.156069	-2.720316
C4	0.000000	0.000000	-2.884554	H10	0.000000	0.000000	-3.972567
C5	0.000000	-1.209960	-2.182383	H11	0.000000	-2.156069	-2.720316
C6	0.000000	-1.217087	-0.783059	H12	0.000000	-2.154443	-0.233507

H_2O $^1A_1$ RB3LYP/6-31+G(d′) C_{2v} Geometry	
Nuclear repulsion energy	9.107110 Hartrees
RB3LYP/6-31+G(d′) energy	-76.417735 Hartrees
Zero-point energy correction	0.021055 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-76.443623 Hartrees

	X	Y	Z		X	Y	Z
O1	-0.000000	0.000000	0.114890	H3	-0.000000	-0.776432	-0.459559
H2	-0.000000	0.776432	-0.459559				

H_2NNH_2 ^1A RB3LYP/6-31+G(d′) C_2 Geometry	
Nuclear repulsion energy	41.526503 Hartrees
RB3LYP/6-31+G(d′) energy	-111.866584 Hartrees
Zero-point energy correction	0.053736 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-111.890942 Hartrees

	X	Y	Z		X	Y	Z
N1	-0.000000	0.714129	-0.071236	H4	0.237980	-1.113618	0.835579
N2	-0.000000	-0.714129	-0.071236	H5	0.926688	1.031185	-0.336927
H3	-0.237980	1.113618	0.835579	H6	-0.926688	-1.031185	-0.336927

$H_2NNH_3^+Br^-$ ^1A RB3LYP/6-31+G(d′) C_1 Geometry	
Nuclear repulsion energy	157.970415 Hartrees
RB3LYP/6-31+G(d′) energy	-2683.891359 Hartrees
Zero-point energy correction	0.065525 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-2683.942665 Hartrees

	X	Y	Z		X	Y	Z
N1	-1.800932	0.679934	-0.000000	H5	-2.120891	1.191954	0.824399
N2	-2.436696	-0.626007	-0.000000	H6	-2.040126	-1.110533	0.808024
H3	-0.641173	0.564581	0.000011	H7	-2.040123	-1.110535	-0.808022
H4	-2.120871	1.191949	-0.824406	Br8	1.103617	-0.031569	0.000000

$B(OH)_3$ $^1A'$ RB3LYP/6-31+G(d′) C_{3h} Geometry	
Nuclear repulsion energy	115.933798 Hartrees
RB3LYP/6-31+G(d′) energy	-252.486459 Hartrees
Zero-point energy correction	0.048275 Hartrees
RB3LYP-D3/6-31+G(2d,p) PCM energy (ε=17.2)	-252.531883 Hartrees

	X	Y	Z		X	Y	Z
B1	0.000000	0.000000	0.000000	H5	-1.059791	-1.642705	-0.000000
O2	0.000000	1.371422	0.000000	O6	1.187686	-0.685711	0.000000
H3	-0.892729	1.739158	0.000000	O7	1.952520	-0.096453	0.000000
O4	-1.187686	-0.685711	0.000000				