Supplementary Information

A Theoretical Study of Ruthenium Complexes with 2,2'-Biimidazole-like Ligands: Structural, Optical and Emissive Properties

Shu-Hua Xia,[†] Wei-Hai Fang,[†] Ganglong Cui,[†] Chantal Daniel[‡]*

[†] *Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, China*

[‡]*Laboratoire de chimie Quantique, Institut de Chimie UMR7177 CNRS-Université de Strasbourg, 1 Rue Blaise Pascal BP 296/R8, F-67008 Strasbourg, France*

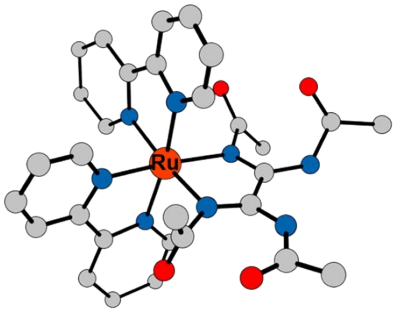

Figure S1. DFT optimized geometry in the electronic ground state of conformer 7b.

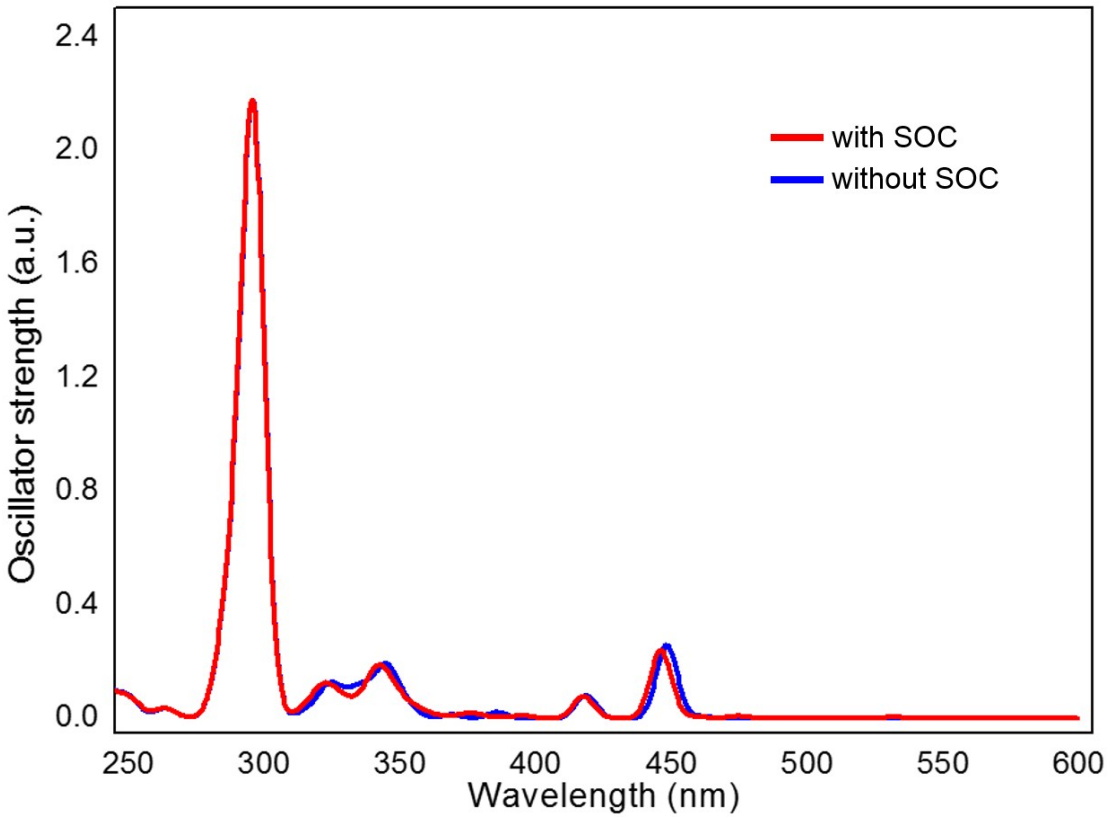

Figure S2. TD-DFT absorption spectrum of $[Ru(bpy)_2(BiimH_2)]^{2+}$ 1 with and without SOC.

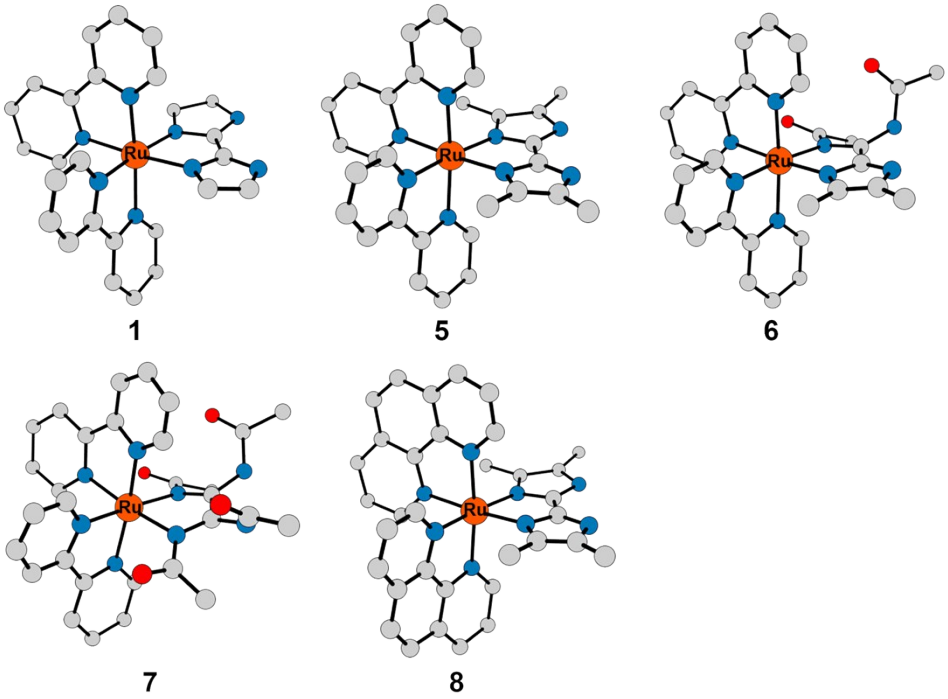

Figure S3. DFT optimized geometries in triplet state of $[Ru(bpy)_2(BiimH_2)]^{2+}$ 1, $[Ru(bpy)_2(TMBiimH_2)^{2+}$ 5, $[Ru(bpy)_2((L1H_2)]^{2+}$ 6, $[Ru(bpy)_2((L2H_2)]^{2+}$ 7 and $[Ru(phen)_2(TMBiimH_2)]^{2+}$ 8.

Table S1. DFT optimized important geometrical parameters of $[Ru(bpy)_2(BiimH_2)]^{2+}$ **1**, $[Ru(bpy)_2(TMBiimH_2)^{2+}$ **5**, $[Ru(bpy)_2((L1H_2)]^{2+}$ **6**, $[Ru(bpy)_2((L2H_2)]^{2+}$ **7** and **7b**, $[Ru(bpy)_2((L2H)]^{+}$ **7d** and $[Ru(phen)_2(TMBiimH_2)]^{2+}$ **8**. Labels of the atoms according to numbering of **1** (complexes **1**, **5** and **8**) and **6** (complexes **6** and **7**) in Figure 1.

	1	5	8		6	7	7b	7d
Ru-N1	2.091	2.090	2.096	Ru-N1	2.092	2.087	2.096	2.080
Ru-N2	2.085	2.082	2.093	Ru-N2	2.084	2.107	2.103	2.092
Ru-N3	2.085	2.082	2.093	Ru-N3	2.079	2.089	2.085	2.087
Ru-N4	2.091	2.090	2.096	Ru-N4	2.100	2.096	2.102	2.100
Ru-N5	2.125	2.147	2.142	Ru-N5	2.114	2.126	2.140	2.144
Ru-N6	2.125	2.147	2.143	Ru-N6	2.164	2.102	2.063	2.148
$N2-C_{15}$	1.343	1.342	1.330	$N6-C_7$	1.440	1.466	1.456	1.419
$C_{15}-C_{16}$	1.384	1.384	1.399	C_8-N9	1.399	1.405	1.403	1.369
$C_{16}-C_{17}$	1.388	1.388	1.375	$N9-C_{10}$	1.385	1.387	1.372	1.320

C_{17}-C_{18}	1.385	1.386	1.407	C_{10}-C_{11}	1.443	1.504	1.481	1.517
C_{18}-C_{19}	1.391	1.392	1.407	N_{12}-C_{11}	-	1.376	1.407	1.366
C_{19}-N2	1.359	1.359	1.365	-	-			-
C_{19}-C_{20}	1.473	1.473	1.427	-	-			-
C_{20}-N1	1.359	1.359	1.365	-	-			-
C_{20}-C_{21}	1.391	1.391	1.407	-	-			-
C_{21}-C_{22}	1.386	1.386	1.407	-	-			-
C_{22}-C_{23}	1.388	1.388	1.375	-	-			-
C_{23}-C_{24}	1.384	1.384	1.400	-	-			-
C_{24}-N_1	1.343	1.343	1.331	-	-			-

Table S2. TD-DFT/B3LYP (without SOC) transition energies (in eV) to the low-lying singlet and triplet excited states of $[Ru(bpy)_2(BiimH_2)]^{2+}$ 1, $[Ru(bpy)_2(TMBiimH_2)^{2+}$ 5, $[Ru(bpy)_2((L1H_2)]^{2+}$ 6, $[Ru(bpy)_2((L2H_2)]^{2+}$ 7 and $[Ru(phen)_2(TMBiimH_2)]^{2+}$ 8 and associated oscillator strengths f.

	Singlet transition energy	f	Triplet transition energy
1 $[Ru(bpy)_2(BiimH_2)]^{2+}$			
	2.46	0.003660	2.34
	2.48	0.000719	2.36
	2.69	0.007603	2.47
	2.72	0.001148	2.54
	2.77	0.257300	2.61
	2.96	0.082109	2.63
	3.21	0.022733	2.90
	3.36	0.013933	3.20
	3.48	0.006733	3.24
	3.52	0.042436	3.27
	3.53	0.001955	3.27
	3.58	0.038148	3.30
	3.59	0.000282	3.30
	3.60	0.089681	3.37

	3.60	0.056600	3.43
	3.69	0.092907	3.44
	3.72	0.008195	3.50
	3.76	0.056053	3.52
	3.83	0.022489	3.53
	3.83	0.075740	3.54
	3.85	0.001066	3.56
	3.85	0.002062	3.58
	3.90	0.002174	3.58
	3.92	0.027995	3.61
	3.99	0.000737	3.66
5 $[Ru(bpy)_2(TMBiimH_2)^{2+}$			
	2.37	0.009336	2.26
	2.38	0.000022	2.28
	2.63	0.001708	2.41
	2.66	0.000524	2.48
	2.71	0.223050	2.55
	2.88	0.066330	2.57
	3.03	0.030176	2.75
	3.09	0.013543	3.01
	3.19	0.046445	3.03
	3.35	0.040777	3.12
	3.45	0.000162	3.21
	3.48	0.008157	3.26
	3.50	0.021566	3.27
	3.58	0.033832	3.28
	3.59	0.088185	3.28
	3.63	0.107920	3.34
	3.70	0.122190	3.39
	3.71	0.043876	3.43
	3.77	0.016632	3.44
	3.77	0.068663	3.47
	3.79	0.004341	3.47
	3.80	0.015701	3.52
	3.81	0.180270	3.54
	3.85	0.000103	3.55
	3.87	0.003875	3.59
6 $[Ru(bpy)_2((L1H_2)]^{2+}$			
	2.24	0.004289	2.04
	2.49	0.006980	2.25
	2.56	0.004747	2.38
	2.65	0.121670	2.43
	2.67	0.116600	2.54
	2.81	0.021722	2.59

	2.89	0.154160	2.71
	2.94	0.054856	2.75
	3.14	0.017102	2.82
	3.46	0.022316	2.83
	3.59	0.167190	3.05
	3.61	0.412380	3.28
	3.69	0.006424	3.29
	3.70	0.004444	3.30
	3.74	0.003167	3.35
	3.75	0.043797	3.37
	3.80	0.023344	3.42
	3.82	0.068924	3.53
	3.87	0.020394	3.57
	3.89	0.009703	3.62
	3.89	0.014174	3.66
	3.93	0.057517	3.68
	3.96	0.019704	3.70
	3.97	0.018584	3.75
	3.98	0.016078	3.77
7 $[Ru(bpy)_2((L2H_2)]^{2+}$			
	1.81	0.002985	1.61
	2.04	0.001170	1.70
	2.46	0.286450	1.89
	2.89	0.001744	2.72
	2.92	0.003020	2.77
	3.13	0.127900	2.88
	3.20	0.006049	2.99
	3.22	0.086206	3.01
	3.26	0.004626	3.08
	3.32	0.002196	3.10
	3.37	0.039805	3.22
	3.53	0.013532	3.24
	3.65	0.001199	3.26
	3.71	0.007435	3.30
	3.73	0.014372	3.35
	3.78	0.004212	3.35
	3.79	0.010515	3.36
	3.93	0.007319	3.43
	3.97	0.051160	3.52
	3.98	0.046868	3.58
	4.00	0.004297	3.61
	4.01	0.020776	3.71
	4.06	0.019376	3.73
	4.06	0.021432	3.79

4.12	0.098623	3.82

7b$[Ru(bpy)_2((L2H_2)]^{2+}$

1.82	0.000527	1.59
1.99	0.001612	1.66
2.60	0.33827	1.83
2.93	0.001856	2.78
3.11	0.002409	2.89
3.12	0.11290	2.89
3.14	0.006799	3.02
3.28	0.08339	3.06
3.31	0.003225	3.09
3.40	0.006391	3.13
3.45	0.020571	3.20
3.48	0.029086	3.22
3.54	0.005009	3.28
3.63	0.003964	3.29
3.66	0.000132	3.29
3.78	0.000368	3.35
3.83	0.007369	3.41
3.89	0.002122	3.47
3.90	0.000656	3.49
4.03	0.047789	3.55
4.05	0.14172	3.66
4.06	0.021950	3.67
4.08	0.023574	3.74
4.11	0.22206	3.83
4.13	0.38138	3.83
4.17	0.16917	3.85

7d $[Ru(bpy)_2((L2H_1)]^{1+}$

2.21	0.005564	1.96
2.45	0.046551	2.12
2.46	0.039684	2.35
2.55	0.038086	2.40
2.59	0.142510	2.42
2.65	0.026068	2.53
2.76	0.062224	2.55
2.85	0.148120	2.61
3.05	0.017664	2.77
3.32	0.010474	2.84
3.36	0.013814	3.06

3.37	0.006382	3.14
3.48	0.002618	3.17
3.54	0.021235	3.21
3.55	0.002172	3.22
3.59	0.030004	3.28
3.64	0.003664	3.28
3.69	0.063093	3.31
3.74	0.093404	3.42
3.77	0.002404	3.44
3.81	0.030062	3.48
3.85	0.025799	3.52
3.86	0.066420	3.58
3.88	0.019638	3.61
3.92	0.014735	3.65
3.93	0.038339	3.70
3.97	0.018154	3.71
3.98	0.000019	3.71
4.04	0.046159	3.76
4.06	0.005588	3.80
4.07	0.021042	3.84
4.11	0.020571	3.92
4.16	0.011968	3.95
4.18	0.303580	3.91
4.20	0.893880	4.04
4.22	0.539080	4.07
4.24	0.106220	4.10

8 $[Ru(phen)_2(TMBiimH_2)]^{2+}$

2.41	0.000429	2.28
2.41	0.016974	2.31
2.68	0.007099	2.41
2.69	0.000581	2.51
2.72	0.000603	2.56
2.72	0.005702	2.60
2.75	0.263650	2.65
2.94	0.026336	2.68
2.98	0.064342	2.77
3.01	0.098470	2.78
3.04	0.062975	2.81
3.04	0.012880	2.93
3.05	0.066784	2.98
3.15	0.085741	3.02
3.28	0.001277	3.05

3.31	0.021147	3.11
3.32	0.091178	3.20
3.59	0.040522	3.23
3.72	0.029833	3.25
3.74	0.006890	3.34
3.79	0.015427	3.36
3.79	0.077816	3.37
3.89	0.038622	3.42
3.96	0.004671	3.49
3.96	0.618440	3.49

Cartesian coordinates of optimized DFT structures in the electronic ground state for the investigated Ru(II) complexes

1 $[Ru(bpy)_2(BiimH_2)]^{2+}$

Ru	-0.16971400	0.00385000	-0.00018600
C	0.44905900	-1.24604400	-2.73991900
H	1.16445700	-0.43902300	-2.79180800
C	0.33026300	-2.16633400	-3.76693600
H	0.96452500	-2.08026600	-4.63538200
C	-0.60789100	-3.18297500	-3.64811700
H	-0.72782300	-3.91983800	-4.42833200
C	-1.39282500	-3.24182500	-2.50769300
H	-2.12213700	-4.02654600	-2.39701600
C	-1.22992300	-2.28710700	-1.50862400
C	-2.01615000	-2.26565900	-0.26301700
C	-3.04160300	-3.16409000	0.01555500
H	-3.30316700	-3.92839600	-0.69668500
C	-3.73172100	-3.06934700	1.21320500
H	-4.52985600	-3.76160400	1.43624500
C	-3.38192900	-2.07138700	2.11279700
H	-3.89123700	-1.95621700	3.05681200
C	-2.35707900	-1.20306100	1.77974000
H	-2.05791100	-0.41195700	2.45055600
C	-2.29011100	1.32505800	-1.77963600
H	-2.03362300	0.51898700	-2.45032500
C	-3.26637200	2.24745600	-2.11327900
H	-3.78063300	2.15995800	-3.05756600
C	-3.56190800	3.26312200	-1.21407800
H	-4.32089500	3.99780900	-1.43787300
C	-2.86815900	3.32073300	-0.01617000
H	-3.08795700	4.09856400	0.69555500
C	-1.89326300	2.36795100	0.26320300

C	-1.10741500	2.34719400	1.50903600
C	-1.22056900	3.30825200	2.50890800
H	-1.90823800	4.12979300	2.39886200
C	-0.43998000	3.20768000	3.64940000
H	-0.52153100	3.94918100	4.43021300
C	0.44396600	2.14345900	3.76743500
H	1.07275000	2.02374800	4.63586300
C	0.51469400	1.21896400	2.73975600
H	1.18704300	0.37569100	2.79113200
C	1.80034900	2.27297600	-1.34197500
C	3.15942100	2.42283800	-1.41496300
C	2.69013300	0.55107400	-0.35851400
C	2.65799400	-0.69102900	0.35715000
C	1.68047600	-2.36402300	1.34173100
C	3.03004000	-2.58316500	1.41598800
N	-0.31057400	-1.29404700	-1.63388600
N	-1.68215300	-1.28940800	0.62222100
N	-1.61204200	1.37503900	-0.62182300
N	-0.24132300	1.30726900	1.63373300
N	1.51621400	1.10146900	-0.68525600
N	3.70290400	1.32939600	-0.79041700
H	4.68766900	1.14898400	-0.68089800
N	1.45716500	-1.18009600	0.68373800
N	3.62926200	-1.51958900	0.79089700
H	4.62205900	-1.39058600	0.68107100
H	1.02972100	2.92258100	-1.71544500
H	3.77124000	3.19300700	-1.84423900
H	3.60130000	-3.38311300	1.84641900
H	0.87712400	-2.97314500	1.71516000

5 $[Ru(bpy)_2(TMBiimH_2)^{2+}$

Ru	-0.14669200	0.00387600	0.00020500
C	0.49179000	-1.25434900	-2.73084800
H	1.22796600	-0.46541100	-2.76739800
C	0.36596000	-2.16739300	-3.76370900
H	1.01450700	-2.09256000	-4.62272000
C	-0.59680300	-3.16274100	-3.66316300
H	-0.72191400	-3.89372200	-4.44791300
C	-1.40000400	-3.20721100	-2.53467600
H	-2.14932300	-3.97494800	-2.43826300
C	-1.23033000	-2.25932700	-1.53020600
C	-2.03768800	-2.22089200	-0.29881400

C	-3.08812100	-3.09581900	-0.03924900
H	-3.35317600	-3.85464400	-0.75614600
C	-3.79989700	-2.98484300	1.14433300
H	-4.61598900	-3.66011600	1.35339500
C	-3.44784500	-1.99091100	2.04738200
H	-3.97518900	-1.86001200	2.97947900
C	-2.39344100	-1.15058600	1.73590900
H	-2.08811300	-0.36796700	2.41399800
C	-2.32969500	1.27431400	-1.73567000
H	-2.06601100	0.47632100	-2.41328800
C	-3.33800100	2.16921500	-2.04774200
H	-3.87140500	2.06600300	-2.97988600
C	-3.63685100	3.18094000	-1.14527800
H	-4.41572900	3.89860600	-1.35503700
C	-2.92058300	3.25449600	0.03852000
H	-3.14510700	4.02702800	0.75477700
C	-1.91819700	2.32506800	0.29880500
C	-1.11033500	2.32080600	1.53046400
C	-1.23044800	3.27603700	2.53512800
H	-1.93868700	4.08184000	2.43872400
C	-0.43104600	3.18932900	3.66385700
H	-0.51797300	3.92573100	4.44872700
C	0.47826100	2.14490300	3.76442200
H	1.12168000	2.03591300	4.62362600
C	0.55631700	1.22666700	2.73144700
H	1.25021400	0.40027900	2.76805300
C	0.81821900	3.15690100	-1.99244600
H	0.14160600	2.62335100	-2.66106700
H	1.28209900	3.96133600	-2.55789500
H	0.21721100	3.60758400	-1.20089700
C	1.85910100	2.24686200	-1.43412900
C	3.23028600	2.35698800	-1.52147700
C	4.11913000	3.36326200	-2.16437500
H	4.76976900	2.89560100	-2.90579600
H	4.75265700	3.85817000	-1.42570200
H	3.52802600	4.12430300	-2.66599800
C	2.71279900	0.53856800	-0.37455100
C	2.68097100	-0.67968100	0.37519200
C	1.73899800	-2.34137500	1.43401000
C	0.65191000	-3.19608800	1.99171400
H	0.02847600	-3.61451500	1.19980200
H	0.00377000	-2.62832800	2.66035100
H	1.07302300	-4.02384500	2.55696300
C	3.10252300	-2.52327600	1.52114800

C	3.93727000	-3.57485200	2.16403000
H	3.30694700	-4.30428500	2.66487400
H	4.61082200	-3.14207900	2.90616100
H	4.54466800	-4.10176000	1.42555200
N	-0.28513900	-1.28810000	-1.63626600
N	-1.69156500	-1.25855000	0.59679800
N	-1.62327800	1.34549900	-0.59647200
N	-0.21746500	1.30125100	1.63665500
N	1.55292800	1.10302600	-0.71534700
N	3.74205100	1.26927600	-0.84567100
H	4.72136000	1.06346500	-0.73153000
N	1.49313900	-1.18273800	0.71579000
N	3.67061100	-1.46361300	0.84573900
H	4.65941600	-1.30970900	0.73116700

6 $[Ru(bpy)_2((L1H_2)]^{2+}$

Ru	0.35797600	0.04424700	-0.01430800
C	-0.95534000	0.95442300	-2.63985700
H	-1.22672400	-0.08849400	-2.70707200
C	-1.35875400	1.86180700	-3.60405000
H	-1.95725500	1.52465100	-4.43581300
C	-0.98170100	3.19071100	-3.46770900
H	-1.28262500	3.92851200	-4.19641300
C	-0.21229600	3.56302800	-2.37638000
H	0.08259500	4.59135200	-2.25231200
C	0.16382300	2.60622400	-1.43987000
C	0.96106100	2.90694200	-0.23831500
C	1.49469900	4.16100200	0.03629700
H	1.35513100	4.97513700	-0.65479700
C	2.21118500	4.36136300	1.20589700
H	2.62807300	5.33238400	1.42771700
C	2.38192300	3.29699900	2.07965200
H	2.93077000	3.40308100	3.00237000
C	1.83678800	2.06868600	1.74633300
H	1.95431500	1.21429500	2.39594600
C	2.77155500	0.09122600	-1.88627900
H	2.09456600	0.64298800	-2.52022000
C	4.08380800	-0.12832200	-2.26615800
H	4.43549700	0.25851200	-3.20974100
C	4.91687600	-0.83848100	-1.41303400
H	5.94830400	-1.02292000	-1.67296700
C	4.40504700	-1.30742300	-0.21373100

H	5.03864200	-1.85440900	0.46393500
C	3.07472300	-1.06249100	0.11159600
C	2.43599000	-1.53523000	1.35086600
C	3.06915100	-2.35880300	2.27599000
H	4.08617000	-2.67509900	2.11591300
C	2.38179800	-2.78246300	3.40218300
H	2.86482300	-3.42379800	4.12387500
C	1.06671100	-2.37540100	3.57809700
H	0.48829900	-2.68542600	4.43431000
C	0.49035900	-1.55556300	2.62330000
H	-0.53175900	-1.22390100	2.72180700
C	0.94206900	-3.17191500	-1.98118200
H	1.32160800	-2.37666300	-2.62282500
H	0.88312800	-4.08250200	-2.57147000
H	1.66840400	-3.33678200	-1.18368000
C	-0.39640900	-2.82525800	-1.42550700
C	-1.58086500	-3.54555300	-1.52333600
C	-1.90047700	-4.84933000	-2.16257600
H	-2.79269300	-4.76874600	-2.78438700
H	-2.08179400	-5.61682700	-1.40751400
H	-1.07589600	-5.17735800	-2.78863700
C	-1.93456600	-1.70303800	-0.35687300
C	-2.49492100	-0.62098800	0.41515900
C	-1.96378500	1.40346700	1.63953200
C	-2.49962200	1.04129500	3.00044300
H	-1.63945700	0.93831800	3.66745800
H	-3.05450300	0.10747800	3.01385200
H	-3.11627500	1.85486200	3.37411600
C	-4.76259100	0.38959900	0.70451600
C	-6.19013400	-0.05921000	0.85088200
H	-6.82827400	0.80851300	0.97953200
H	-6.29560300	-0.72765100	1.70629800
H	-6.49500300	-0.60381300	-0.04486700
N	-0.21277700	1.30915700	-1.58024900
N	1.14199000	1.86918900	0.61745100
N	2.26806300	-0.36310800	-0.72793000
N	1.15061100	-1.13189000	1.53467600
N	-0.64205000	-1.68748800	-0.70138100
N	-2.52138900	-2.81742200	-0.85468900
H	-3.49116200	-3.07928900	-0.77628100
N	-1.64614900	0.31078000	0.75641800
N	-3.84793300	-0.66916300	0.70909700
H	-4.26429400	-1.58797800	0.71081300
O	-1.63671400	2.52814900	1.33982000

O	-4.40303200	1.54550900	0.58610200

7b $[Ru(bpy)_2((L2H_2)]^{2+}$

Ru	0.51584100	-0.00510300	-0.03782900
C	1.09561500	-1.22051600	2.74209000
H	0.11903000	-0.82585100	2.97461900
C	1.85617000	-1.85362200	3.70939200
H	1.46913000	-1.95333600	4.71108900
C	3.10759200	-2.34085900	3.35994200
H	3.73362800	-2.83151700	4.08966600
C	3.54519400	-2.19572200	2.05296900
H	4.50877600	-2.57882100	1.76277200
C	2.73458800	-1.55563100	1.12193300
C	3.09646900	-1.38344100	-0.29516400
C	4.30164300	-1.80941100	-0.84104400
H	5.04825000	-2.27139900	-0.21788600
C	4.54219000	-1.63064300	-2.19436200
H	5.47795100	-1.95280800	-2.62545200
C	3.56585700	-1.03452900	-2.97880300
H	3.70623700	-0.87753400	-4.03651600
C	2.38864200	-0.62063900	-2.37960500
H	1.61173600	-0.13828400	-2.95246400
C	2.56591300	1.94255400	1.17351500
H	2.69785300	1.15153700	1.89554500
C	3.30166500	3.11173800	1.26562500
H	4.01286300	3.23022500	2.06800100
C	3.10257900	4.10124000	0.31456500
H	3.66041300	5.02493500	0.35031400
C	2.16786400	3.89058400	-0.68656200
H	1.99760200	4.64996800	-1.43059800
C	1.44951900	2.70114400	-0.72010200
C	0.40081700	2.41574200	-1.71256700
C	-0.01091400	3.32850800	-2.67672600
H	0.45138600	4.29877800	-2.73898900
C	-1.03216700	2.99179600	-3.55107100
H	-1.36141400	3.69804100	-4.29825000
C	-1.62232500	1.74125200	-3.44532000
H	-2.42173100	1.43355600	-4.10098500
C	-1.17094000	0.87171900	-2.46756500
H	-1.60946900	-0.10826600	-2.35979600
C	-1.49276900	1.62824000	3.31822200
H	-2.15608400	0.79081300	3.51786400

H	-1.90736800	2.54633000	3.72656900
H	-0.53806700	1.44032100	3.81666600
C	-1.20558100	1.82374000	1.85614900
C	-4.25556500	1.18607200	1.55014500
C	-5.70861800	0.95594200	1.84807700
H	-5.81926300	0.26440800	2.68438300
H	-6.19486900	0.51442600	0.97544500
H	-6.18253300	1.90270000	2.08407000
C	-2.25399000	-0.16772400	0.91426600
C	-2.00248600	-1.41982000	0.16401500
C	-0.49463400	-2.73173800	-1.13688400
C	0.17595400	-3.84457300	-0.40221800
H	0.27022100	-4.70836800	-1.05285100
H	-0.37992100	-4.10116000	0.50036200
H	1.16926600	-3.52183200	-0.08269500
C	-3.95408300	-2.27306600	-1.02776900
C	-4.80816600	-3.49339100	-1.22066200
H	-5.73633800	-3.21191000	-1.70867800
H	-5.01480000	-3.99555200	-0.27696900
H	-4.26879600	-4.18931400	-1.86784100
N	1.52089600	-1.05660200	1.47970400
N	2.15398900	-0.78176800	-1.06832000
N	1.66068900	1.73338700	0.20669300
N	-0.18252500	1.19332900	-1.61807800
N	-1.22647600	0.62131700	1.03546000
N	-3.52932500	-0.00366700	1.39220400
H	-4.08119700	-0.85120500	1.37028800
N	-0.81364600	-1.55700600	-0.31965700
N	-3.02064900	-2.37766400	0.00007300
H	-2.90106300	-3.27456800	0.45228500
O	-0.73603000	-2.68933100	-2.31528400
O	-4.02714500	-1.25246500	-1.69355800
O	-3.72480600	2.27320200	1.43838900
O	-0.79320300	2.85084000	1.37927600

7 $[Ru(bpy)_2((L2H_2)]^{2+}$

Ru	0.499864	0.076047	-0.089287
C	0.966411	-1.347822	2.598518
H	0.044688	-0.855555	2.866624
C	1.610922	-2.181710	3.495041
H	1.188938	-2.338221	4.475237
C	2.789253	-2.799524	3.100638

H	3.320178	-3.458385	3.771338
C	3.276354	-2.563926	1.824871
H	4.184649	-3.041881	1.499357
C	2.580987	-1.719442	0.966835
C	3.005162	-1.430920	-0.412716
C	4.172962	-1.927371	-0.981814
H	4.830262	-2.559229	-0.409020
C	4.491986	-1.600591	-2.290658
H	5.396296	-1.981885	-2.739747
C	3.636274	-0.775489	-3.007675
H	3.844877	-0.487106	-4.026586
C	2.488581	-0.312644	-2.389830
H	1.800233	0.335043	-2.911458
C	2.562129	1.913889	1.231056
H	2.664276	1.083527	1.912864
C	3.345864	3.047024	1.367839
H	4.066377	3.100940	2.168642
C	3.186965	4.081996	0.458018
H	3.787807	4.976596	0.525548
C	2.240845	3.953466	-0.546621
H	2.104504	4.746807	-1.261755
C	1.472572	2.797872	-0.624556
C	0.416731	2.589278	-1.628766
C	0.015565	3.563866	-2.535137
H	0.494892	4.527911	-2.543170
C	-1.018035	3.297251	-3.419179
H	-1.339883	4.051993	-4.120911
C	-1.631893	2.053800	-3.380927
H	-2.443583	1.800608	-4.044342
C	-1.184741	1.122219	-2.460689
H	-1.636337	0.143934	-2.402897
C	-1.696368	1.616004	3.233997
H	-2.291468	0.722053	3.392353
H	-2.234650	2.498021	3.575292
H	-0.782257	1.538282	3.828879
C	-1.278379	1.819477	1.805000
C	-4.226387	1.393069	1.045426
C	-5.643380	1.374120	1.551258
H	-5.721153	0.850664	2.502166
H	-6.271966	0.850253	0.824105
H	-6.000336	2.390404	1.656995
C	-2.272709	-0.135102	0.783496
C	-2.036546	-1.401835	0.008151
C	-0.253162	-2.678240	-1.150096

C	-0.391533	-2.639427	-2.639783
H	-0.057245	-3.590405	-3.051984
H	0.241619	-1.840404	-3.036763
H	-1.420675	-2.438048	-2.933847
C	-3.265248	-3.509273	-0.670291
C	-4.662024	-4.047746	-0.592651
H	-4.748970	-4.894676	-1.259288
H	-5.409456	-3.305693	-0.848736
H	-4.847793	-4.380747	0.433174
N	1.434271	-1.110649	1.363987
N	2.167893	-0.635351	-1.126122
N	1.647515	1.784023	0.259578
N	-0.183994	1.371523	-1.603869
N	-1.236007	0.620471	0.963137
N	-3.564459	0.162389	1.191965
H	-4.083749	-0.564525	1.655086
N	-0.832409	-1.542343	-0.443856
N	-3.135062	-2.216014	-0.143946
H	-4.011118	-1.767957	0.070066
O	0.443428	-3.445717	-0.530161
O	-2.311034	-4.128845	-1.100332
O	-3.676388	2.344886	0.525372

7d $[Ru(bpy)_2((L2H)]^+$

Ru	0.477611	0.103152	-0.208689
C	0.802460	-1.307914	2.514495
H	-0.123234	-0.798260	2.733071
C	1.402835	-2.132364	3.450108
H	0.942380	-2.267036	4.416401
C	2.589307	-2.769618	3.114506
H	3.085829	-3.421860	3.817120
C	3.130672	-2.558786	1.856561
H	4.046826	-3.050359	1.575982
C	2.482688	-1.715515	0.959796
C	2.984441	-1.426342	-0.394354
C	4.197226	-1.899813	-0.885548
H	4.826830	-2.520982	-0.271441
C	4.599375	-1.560317	-2.167094
H	5.539608	-1.921505	-2.555049
C	3.777816	-0.746933	-2.935494
H	4.049519	-0.451034	-3.936605
C	2.583217	-0.306691	-2.394699
H	1.916205	0.325307	-2.960812

C	2.531004	1.929083	1.137397
H	2.615920	1.102735	1.826724
C	3.319369	3.058310	1.280482
H	4.027760	3.113228	2.092382
C	3.180408	4.090155	0.363001
H	3.784794	4.982040	0.435858
C	2.249471	3.959820	-0.655400
H	2.128458	4.749524	-1.377628
C	1.476460	2.807078	-0.739462
C	0.441734	2.593946	-1.764425
C	0.058880	3.563905	-2.684819
H	0.534470	4.530155	-2.686311
C	-0.951739	3.289025	-3.592629
H	-1.259668	4.038829	-4.305879
C	-1.561488	2.042514	-3.561641
H	-2.356821	1.783563	-4.242840
C	-1.135399	1.117522	-2.624386
H	-1.588296	0.139662	-2.563988
C	-1.746799	1.684368	3.107691
H	-2.287739	0.759226	3.285953
H	-2.354072	2.535392	3.410856
H	-0.842060	1.687500	3.720073
C	-1.309534	1.863566	1.671528
C	-4.271278	1.203525	1.404837
C	-5.506130	1.014705	2.254421
H	-5.259430	0.455693	3.158319
H	-6.243012	0.429020	1.701510
H	-5.935988	1.976994	2.518926
C	-2.362620	-0.061479	0.698547
C	-2.078393	-1.341121	-0.065458
C	-0.407640	-2.779153	-1.028345
C	0.126428	-2.833612	-2.429493
H	-0.140067	-3.794436	-2.862042
H	1.215026	-2.769940	-2.396596
H	-0.256615	-2.027083	-3.047691
C	-3.459597	-3.155956	-1.063959
C	-4.793408	-3.809244	-0.833862
H	-5.010815	-4.488689	-1.650944
H	-5.579923	-3.056581	-0.760535
H	-4.768982	-4.361832	0.107394
N	1.322976	-1.092194	1.296517
N	2.182919	-0.637087	-1.156245
N	1.631124	1.796216	0.152422
N	-0.155256	1.374149	-1.745383

N	-1.293391	0.711347	0.843937
N	-3.603678	0.039314	1.136520
N	-0.898796	-1.500650	-0.570287
N	-3.143725	-2.195159	-0.112488
H	-3.903397	-1.832554	0.462688
O	-0.319323	-3.693964	-0.237161
O	-2.706199	-3.425351	-1.986535
O	-3.961329	2.311783	0.951236
O	-0.833640	2.913855	1.283583

8 $[Ru(phen)_2(TMBiimH_2)]^{2+}$

Ru	-0.10698200	0.00187300	-0.00238400
C	0.50109500	-1.35281100	-2.72968200
H	1.27471600	-0.60389300	-2.81559000
C	0.30793600	-2.30631600	-3.73568400
H	0.94915800	-2.28866000	-4.60310600
C	-0.69222200	-3.24168300	-3.60626900
H	-0.86271100	-3.98192200	-4.37414100
C	-1.50174100	-3.22721800	-2.45553100
C	-1.23308200	-2.24435100	-1.48496900
C	-2.01060700	-2.18736200	-0.28949100
C	-3.07006800	-3.09288400	-0.09409500
C	-3.81525900	-2.97518400	1.09318200
H	-4.63919200	-3.64793000	1.28006200
C	-3.48179800	-1.99660300	2.00040600
H	-4.03381200	-1.87168000	2.91868700
C	-2.40443400	-1.14423200	1.73608300
H	-2.12269100	-0.37722600	2.44246800
C	-2.34237700	1.27228300	-1.73544600
H	-2.10364900	0.49196700	-2.44319400
C	-3.37298000	2.18173400	-1.99646200
H	-3.93300100	2.08769400	-2.91364600
C	-3.65161700	3.17565700	-1.08741400
H	-4.43884800	3.89189600	-1.27169500
C	-2.89845500	3.25178200	0.09825900
C	-1.88888800	2.29034900	0.29034600
C	-1.10674400	2.30441500	1.48408800
C	-1.31992100	3.29947300	2.45601200
C	-0.50885600	3.26887200	3.60538700
H	-0.63788100	4.01629300	4.37441700

C	0.43930800	2.28051100	3.73210100
H	1.07969900	2.22676800	4.59866800
C	0.57905900	1.31927200	2.72456500
H	1.31096500	0.52934400	2.80854100
C	0.84522600	3.13250500	-2.01925000
H	0.17644200	2.59370100	-2.69167100
H	1.30450600	3.94240100	-2.58071600
H	0.23682600	3.57635600	-1.22929100
C	1.89041200	2.23050600	-1.45631400
C	3.26139200	2.35148000	-1.53343900
C	4.14620600	3.36966100	-2.16312700
H	4.83440600	2.90749100	-2.87415700
H	4.74089600	3.89356000	-1.41117300
H	3.55266600	4.10671200	-2.69753700
C	2.74998600	0.53069800	-0.38705900
C	2.71838700	-0.67781500	0.37860300
C	1.77102100	-2.32686100	1.45323800
C	0.68027100	-3.17127100	2.01940100
H	0.05488100	-3.59349200	1.23072900
H	0.03495600	-2.59366700	2.68225600
H	1.09660600	-3.99658000	2.59157200
C	3.13379500	-2.51967600	1.53012600
C	3.96378100	-3.58026500	2.16438200
H	3.33291700	-4.28219900	2.70292500
H	4.67597600	-3.15172700	2.87196500
H	4.52861800	-4.13881800	1.41510500
N	-0.24813600	-1.31043700	-1.63091700
N	-1.67470300	-1.23390500	0.62761400
N	-1.60679700	1.32109000	-0.62839000
N	-0.17316200	1.31875800	1.62699800
N	1.58850900	1.08545300	-0.73880900
N	3.77671500	1.26873100	-0.85199200
H	4.75691200	1.07456800	-0.72516900
N	1.52944700	-1.16992900	0.73177800
N	3.70518200	-1.46729600	0.84574300
H	4.69425900	-1.32554900	0.71796100
C	-2.34296700	4.27426600	2.23037500
C	-3.10268300	4.24692500	1.10621700
H	-2.50332100	5.03403400	2.98065800
H	-3.87728400	4.98311200	0.95082600
C	-3.33017800	-4.07602900	-1.10097800
C	-2.57582600	-4.14482600	-2.22693500
H	-2.77967500	-4.89497300	-2.97635800
H	-4.14312000	-4.76941300	-0.94413100

Cartesian coordinates of all optimized DFT structures in triplet state

1 $[Ru(bpy)_2(BiimH_2)]^{2+}$

Ru	-0.15489600	0.01369700	0.00328700
C	0.51163100	-1.32596600	-2.70129600
H	1.23925700	-0.53066800	-2.75623400
C	0.40178300	-2.26965400	-3.70727700
H	1.05677100	-2.21545500	-4.56206200
C	-0.55525100	-3.26702600	-3.58373100
H	-0.66706800	-4.02189300	-4.34751500
C	-1.37227200	-3.28743400	-2.46428300
H	-2.11655200	-4.05753300	-2.35406400
C	-1.22091800	-2.30969900	-1.48817000
C	-2.03648500	-2.24059900	-0.26462600
C	-3.07544000	-3.11732100	0.02261000
H	-3.32746200	-3.90629400	-0.66508300
C	-3.79107500	-2.96730500	1.20030700
H	-4.59976500	-3.64445400	1.43046600
C	-3.45771600	-1.93970600	2.07096700
H	-3.98920400	-1.78625900	2.99652900
C	-2.41767300	-1.09219400	1.73342000
H	-2.12131100	-0.27770100	2.37621800
C	-2.31418300	1.26262700	-1.77235000
H	-2.06010200	0.44786000	-2.43507000
C	-3.29939800	2.15751400	-2.10599500
H	-3.82975800	2.04988500	-3.03898200
C	-3.58923600	3.20788500	-1.19877300
H	-4.36347700	3.92649400	-1.42719900
C	-2.89128200	3.30294900	-0.02711800
H	-3.11681300	4.09136000	0.67296200
C	-1.87612000	2.36222500	0.28701300
C	-1.11782300	2.34889300	1.48005700
C	-1.19550600	3.32027800	2.51174200
H	-1.88696100	4.14185300	2.41340300
C	-0.39747400	3.22686700	3.61729800
H	-0.46356300	3.97262200	4.39672200
C	0.52319200	2.15201700	3.73217500
H	1.16828300	2.04647700	4.59009000
C	0.57773900	1.23093900	2.71842300
H	1.25904600	0.39348600	2.76356300
C	1.75285300	2.35871600	-1.18495300

C	3.10708900	2.54336400	-1.23006900
C	2.68873900	0.58043000	-0.33058700
C	2.67177800	-0.69523100	0.31834500
C	1.69435600	-2.43710000	1.18911400
C	3.04328400	-2.66805900	1.21303100
N	-0.28023700	-1.34060000	-1.61954300
N	-1.72007000	-1.24036700	0.59724600
N	-1.59966200	1.34731000	-0.62985700
N	-0.21806700	1.28925700	1.62729100
N	1.50133200	1.12824200	-0.63228500
N	3.67488100	1.41828600	-0.68653900
H	4.66352700	1.26240300	-0.56883100
N	1.47207500	-1.20127000	0.63757800
N	3.63817900	-1.56367700	0.66047600
H	4.62939900	-1.43957400	0.52741200
H	0.96530900	3.01121900	-1.51434500
H	3.70260500	3.35798100	-1.59505300
H	3.61664100	-3.50196600	1.57005400
H	0.89518600	-3.06592400	1.53641600

5 $[Ru(bpy)_2(TMBiimH_2)^{2+}$

Ru	0.10347800	0.02282300	0.00205200
C	-0.63270800	-1.50155800	2.58729900
H	-1.37494100	-0.72210800	2.66612000
C	-0.54682500	-2.51024900	3.53067200
H	-1.23545300	-2.52393000	4.36034200
C	0.42818300	-3.48541000	3.37637700
H	0.51918100	-4.29182700	4.08836200
C	1.28902100	-3.41702900	2.29200200
H	2.04672800	-4.16987200	2.15661200
C	1.16161200	-2.37550300	1.38067600
C	2.02068600	-2.21416200	0.19683900
C	3.11750000	-3.02274400	-0.07686000
H	3.38584000	-3.82090200	0.59407200
C	3.87179200	-2.79025500	-1.21637200
H	4.72642000	-3.41217500	-1.43545400
C	3.51696800	-1.74888500	-2.06164000
H	4.07607400	-1.53077300	-2.95755300
C	2.42040000	-0.97013800	-1.73560900
H	2.10914300	-0.14631300	-2.35919600
C	2.36651900	1.06064600	1.79108900
H	2.04791400	0.25943800	2.44277500

C	3.44854800	1.84053300	2.11830600
H	3.98856100	1.65331000	3.03310800
C	3.82282500	2.87661100	1.22774400
H	4.67527600	3.50350300	1.44737000
C	3.10585200	3.07241100	0.07958800
H	3.39550000	3.84834500	-0.61104600
C	1.98871000	2.25188100	-0.22247700
C	1.19818700	2.35091800	-1.39210100
C	1.32645900	3.35655500	-2.38368600
H	2.08356100	4.11619600	-2.27154800
C	0.49311900	3.37767000	-3.46715800
H	0.59805500	4.15034200	-4.21536100
C	-0.51658400	2.38737100	-3.59758600
H	-1.19230200	2.37297500	-4.43821800
C	-0.61871600	1.43053800	-2.62198600
H	-1.36798600	0.65448100	-2.67979500
C	-0.70319600	3.18101900	1.95293700
H	-0.05752000	2.63503600	2.64150100
H	-1.13464700	4.02252100	2.48833300
H	-0.07725100	3.57307300	1.15024100
C	-1.78191900	2.30602200	1.41471600
C	-3.14748800	2.47579100	1.49041700
C	-3.98974200	3.53466100	2.10653600
H	-4.65232300	3.11342900	2.86462200
H	-4.60743100	4.02793900	1.35395400
H	-3.36506200	4.28650200	2.57972600
C	-2.72203900	0.60436600	0.39307000
C	-2.72947000	-0.60291100	-0.36437000
C	-1.80773900	-2.29294300	-1.40912400
C	-0.73485600	-3.15882200	-1.97462300
H	-0.14671300	-3.63062100	-1.18538600
H	-0.05608800	-2.58356100	-2.60472300
H	-1.16715600	-3.94964500	-2.58178800
C	-3.17525500	-2.47361200	-1.45249000
C	-4.02282300	-3.54209300	-2.04457100
H	-3.40596600	-4.26809000	-2.56604100
H	-4.73660300	-3.12452300	-2.75643200
H	-4.58546100	-4.06681500	-1.27025200
N	0.19865300	-1.43215200	1.53799500
N	1.68602800	-1.19825700	-0.63753700
N	1.63301200	1.24983500	0.67631600
N	0.20885900	1.37531600	-1.55360700
N	-1.53290400	1.12729300	0.73399600
N	-3.70797700	1.39608000	0.83899900

H	-4.69619600	1.23920800	0.71819400
N	-1.54847400	-1.11722200	-0.73284400
N	-3.72504200	-1.39907900	-0.78793800
H	-4.71112900	-1.24607100	-0.64647100

6 $[Ru(bpy)_2((L1H_2)]^{2+}$

Ru	0.35893100	0.02075500	0.08237100
C	-1.19041500	0.94595600	-2.38704800
H	-1.44612000	-0.10021300	-2.44327100
C	-1.68413800	1.85907300	-3.30073200
H	-2.33874600	1.52190600	-4.08849700
C	-1.33055200	3.19309200	-3.16688400
H	-1.70813300	3.93508800	-3.85426600
C	-0.48308100	3.57127500	-2.13567500
H	-0.20331200	4.60425800	-2.01826300
C	-0.00251400	2.61149000	-1.25579000
C	0.91772200	2.90222300	-0.14653100
C	1.47109000	4.15425400	0.09056500
H	1.23475500	4.98495800	-0.55218100
C	2.33860500	4.32644100	1.15760400
H	2.77531800	5.29488200	1.34943600
C	2.63808500	3.24078400	1.96678200
H	3.30888800	3.32643300	2.80651900
C	2.06006400	2.01676300	1.67743000
H	2.26448700	1.14926500	2.28602800
C	2.73096500	0.19528900	-1.87649500
H	2.02745300	0.77997500	-2.44943000
C	4.02504700	-0.00370300	-2.32363500
H	4.33780600	0.43469700	-3.25777900
C	4.88792300	-0.76398500	-1.54776100
H	5.90584000	-0.93585500	-1.86290000
C	4.42984700	-1.30174700	-0.35484600
H	5.09013400	-1.88846500	0.26063700
C	3.11683400	-1.07392100	0.04010000
C	2.53067400	-1.59778900	1.28406700
C	3.20170500	-2.44333200	2.15795300
H	4.21112400	-2.75341800	1.94776000
C	2.56194400	-2.89036400	3.30418900
H	3.07703200	-3.54771100	3.98799200
C	1.25916100	-2.48562900	3.55488800
H	0.72445000	-2.80949400	4.43352900
C	0.63603200	-1.64873200	2.64641800

H	-0.37710700	-1.30947100	2.79402700
C	0.96543800	-3.17310400	-1.94594100
H	1.31740700	-2.37147400	-2.59723500
H	0.89778600	-4.08006200	-2.54066900
H	1.71953900	-3.33778200	-1.17416700
C	-0.35985100	-2.84665100	-1.34824100
C	-1.54201700	-3.54964800	-1.44516400
C	-1.89372200	-4.82020900	-2.13100300
H	-2.67793900	-4.65898400	-2.87299100
H	-2.25730900	-5.56001500	-1.41542300
H	-1.02622200	-5.23536900	-2.63604600
C	-1.88914500	-1.73745600	-0.20057100
C	-2.42189300	-0.72681200	0.61138600
C	-1.82480400	1.20526800	1.96574300
C	-2.88928000	0.93092400	3.01188800
H	-2.56301200	1.41334500	3.93220900
H	-3.04854400	-0.12829800	3.19660000
H	-3.83856200	1.38180100	2.71682300
C	-4.56589800	0.33081100	0.06112000
C	-6.05352400	0.26040600	0.31713500
H	-6.42262600	1.25961000	0.54683700
H	-6.31371000	-0.41776000	1.12744700
H	-6.54386200	-0.07799400	-0.59719600
N	-0.36789000	1.30874400	-1.39251900
N	1.22133400	1.85037700	0.64921500
N	2.28443800	-0.32929000	-0.72721100
N	1.25420400	-1.21049500	1.54034100
N	-0.59215900	-1.71655200	-0.58604700
N	-2.48319500	-2.83152400	-0.73195300
H	-3.44332500	-3.10117600	-0.59226400
N	-1.51439100	0.23433700	1.02978300
N	-3.81947800	-0.60496900	0.73748200
H	-4.30971800	-1.22705000	1.36246200
O	-1.19145300	2.26308500	2.01414100
O	-4.05270700	1.15262900	-0.69244300

7 $[Ru(bpy)_2((L2H_2)]^{2+}$

Ru	0.63519300	-0.02252200	0.07942900
C	1.43543400	-1.37927600	2.70869300
H	0.50528800	-0.95090100	3.04701900
C	2.23104800	-2.12982000	3.55371100
H	1.92058900	-2.29075600	4.57353800

C	3.41461800	-2.65954600	3.05793300
H	4.05855700	-3.25316100	3.68885500
C	3.76520300	-2.42240800	1.73792400
H	4.67799700	-2.83129400	1.33972600
C	2.93084600	-1.65711000	0.93327100
C	3.20120600	-1.35443500	-0.47908600
C	4.34357500	-1.76295900	-1.15462400
H	5.10541400	-2.32722500	-0.64458800
C	4.49829000	-1.43725000	-2.49336700
H	5.38275100	-1.75051800	-3.02702800
C	3.50773300	-0.70569100	-3.13191100
H	3.58527100	-0.43084900	-4.17163500
C	2.39698800	-0.31484400	-2.40548700
H	1.60634100	0.25955200	-2.86233700
C	2.77227100	1.98656100	0.96731400
H	3.12697400	1.14800700	1.54593800
C	3.38742400	3.22219300	1.05602400
H	4.24116700	3.34553900	1.70295700
C	2.87845900	4.27464000	0.30949700
H	3.32930100	5.25420100	0.35890100
C	1.78119600	4.05588900	-0.50903100
H	1.38022500	4.86076000	-1.10086200
C	1.20579500	2.79292000	-0.55966100
C	0.05868500	2.44957800	-1.41199100
C	-0.58177700	3.35615400	-2.24684000
H	-0.26658800	4.38512000	-2.27492400
C	-1.62901800	2.92869200	-3.04773100
H	-2.13400800	3.62836200	-3.69608000
C	-2.00676600	1.59457300	-3.01324700
H	-2.80120200	1.21454100	-3.63616900
C	-1.34371400	0.73402900	-2.15613100
H	-1.60119600	-0.31518800	-2.11257100
C	-1.94650900	1.32392500	3.50682900
H	-2.44060700	0.35793500	3.55369200
H	-2.70030100	2.10714300	3.42000000
H	-1.39449300	1.49931200	4.42814800
C	-0.95710300	1.44596800	2.36758400
C	-3.77638700	1.64411300	0.88506200
C	-5.27172000	1.81492000	0.85288500
H	-5.71796600	1.41397300	1.76416500
H	-5.69115900	1.27037300	0.00452700
H	-5.51138500	2.86869700	0.75819800
C	-2.09997600	-0.18151800	0.96298000
C	-1.89247900	-1.41219400	0.29571000

C	-0.17140500	-3.02174600	-0.31701000
C	-0.85277000	-4.18866800	0.36117300
H	-1.55367300	-4.66401600	-0.32665600
H	-1.38130500	-3.90695500	1.26796700
H	-0.08063700	-4.91810500	0.59581700
C	-3.24803100	-2.69032800	-1.32981700
C	-4.45195600	-3.58738200	-1.43156600
H	-5.05354200	-3.26990200	-2.28110700
H	-5.05954300	-3.58833900	-0.52994700
H	-4.10732700	-4.60441100	-1.62704200
N	1.77614700	-1.14200600	1.43243800
N	2.24608300	-0.63229000	-1.11393700
N	1.70479200	1.77826800	0.18712300
N	-0.34522600	1.15355300	-1.36213100
N	-0.99614500	0.50470400	1.32249500
N	-3.38242400	0.31700500	1.12235600
H	-4.13058300	-0.35620000	1.05949700
N	-0.61974400	-1.71002900	-0.05823000
N	-2.98539700	-2.21330400	-0.05372100
H	-3.61634900	-2.50524000	0.67778000
O	0.81492200	-3.18948400	-1.01687000
O	-2.53909300	-2.39925800	-2.28195500
O	-2.97140300	2.54186100	0.73071900
O	-0.04981200	2.26179400	2.41093800

8 $[Ru(phen)_2(TMBiimH_2)]^{2+}$

Ru	-0.04920200	0.03229400	0.00362500
C	0.59207600	-1.44676400	-2.67603200
H	1.38931800	-0.72393900	-2.76368000
C	0.38724100	-2.41613900	-3.66313300
H	1.04425600	-2.43915900	-4.51775900
C	-0.64525000	-3.31459500	-3.52961900
H	-0.82305200	-4.06757000	-4.28296000
C	-1.48080900	-3.24883700	-2.39911800
C	-1.20469900	-2.24878800	-1.44976900
C	-2.00887300	-2.13322700	-0.27864200
C	-3.09819900	-3.00133800	-0.08339100
C	-3.86511200	-2.82421900	1.08313700
H	-4.71149600	-3.46820400	1.27024700
C	-3.52767300	-1.82967800	1.97050200
H	-4.09602700	-1.66516200	2.87193700
C	-2.42363000	-1.01157000	1.70729700

H	-2.13261200	-0.22817700	2.39115200
C	-2.30679100	1.24416100	-1.76880900
H	-2.03918700	0.47878800	-2.48395900
C	-3.36118700	2.10673300	-2.02383900
H	-3.91456000	2.00300200	-2.94390700
C	-3.68324500	3.09877400	-1.08680800
H	-4.49906800	3.78325000	-1.27113200
C	-2.94980800	3.19567700	0.08716600
C	-1.88204900	2.27284500	0.29473200
C	-1.12865600	2.29219300	1.46425700
C	-1.36148500	3.27024800	2.47064000
C	-0.55043100	3.26648900	3.59723400
H	-0.70389900	3.99676900	4.37863200
C	0.48162400	2.30281900	3.70649200
H	1.13153900	2.28078600	4.56752800
C	0.65355300	1.37015900	2.71460500
H	1.42128700	0.61376400	2.78518000
C	0.83530300	3.19633200	-1.89132500
H	0.18121400	2.69017400	-2.60187700
H	1.29053700	4.04387400	-2.39634700
H	0.21479100	3.57858100	-1.07976600
C	1.88884400	2.27789500	-1.37610300
C	3.25826400	2.40651500	-1.45697100
C	4.12903300	3.44881000	-2.06108000
H	4.76824000	3.02108500	-2.83546300
H	4.77131100	3.90480200	-1.30563800
H	3.52506600	4.23099200	-2.51139300
C	2.78361000	0.53268100	-0.38436500
C	2.75516100	-0.68463600	0.35456700
C	1.77812600	-2.35775000	1.37666400
C	0.67854800	-3.19510700	1.93354900
H	0.05979400	-3.61825700	1.14032100
H	0.03412400	-2.61108800	2.59101700
H	1.08607200	-4.02055000	2.51058100
C	3.13921700	-2.58769000	1.40824400
C	3.95058600	-3.69745200	1.97421200
H	3.31028800	-4.41422300	2.47995100
H	4.67891600	-3.32063500	2.69401100
H	4.49387200	-4.22252800	1.18643400
N	-0.18296100	-1.35937200	-1.60005100
N	-1.67817900	-1.16327600	0.61832400
N	-1.56172400	1.31649700	-0.65889500
N	-0.14002700	1.31856900	1.61368300
N	1.60784000	1.09677000	-0.71132500

N	3.78965600	1.30015300	-0.82475400
H	4.77346400	1.11189000	-0.71276000
N	1.55803200	-1.16301600	0.72134700
N	3.72373900	-1.52257200	0.75914300
H	4.71381000	-1.40393500	0.61233000
C	-2.43245900	4.20412500	2.24300300
C	-3.18908100	4.16447500	1.11787000
H	-2.62753900	4.94887000	3.00131900
H	-3.99218300	4.87374000	0.97709200
C	-3.36284900	-4.00614600	-1.06618900
C	-2.58556300	-4.12830400	-2.17200600
H	-2.79304600	-4.89291400	-2.90537600
H	-4.19827800	-4.67125800	-0.90824400