Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Supporting Information for

Photophysical and electrochemical properties of polypyridine imine ruthenium(II) complexes: a comparative experimental and theoretical study.

Rémi E. Piau,[a] Thomas Guillon,[a] Emilie Lebon,[b] Nicolas Perrot,[b] Fabienne Alary,*[a] Martial Boggio-Pasqua,[a] Jean-Louis Heully,[a] Alberto Juris,[c] Pierre Sutra[b] and Alain Igau*[b]

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Figure S1. Cyclic voltammogram of $[Ru(bpy)_2(Mes\text{-}dab)]^{2+}$ at 100 mV/s scan rate, in acetonitrile solution with $[Bu_4N]PF_6$ as supporting electrolyte.

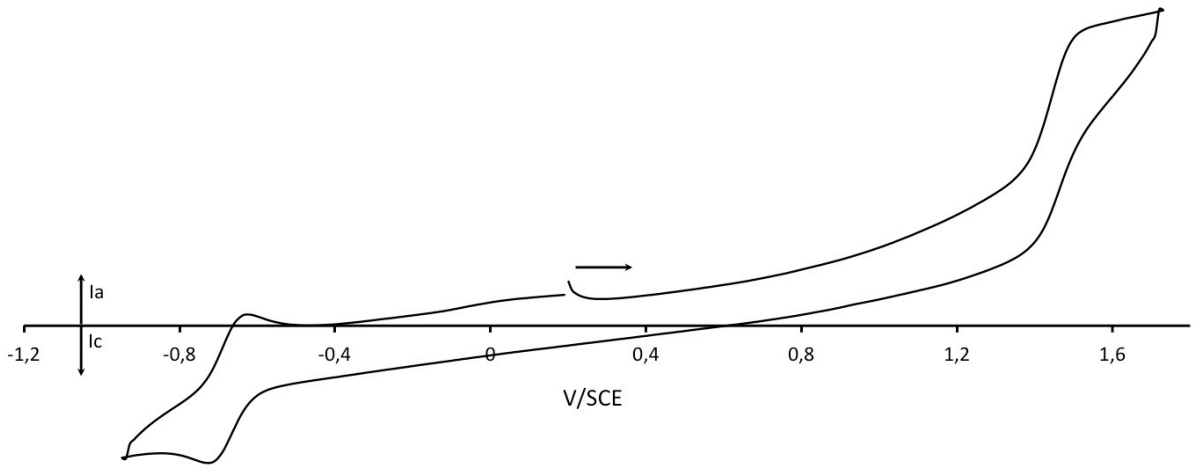

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Figure S2. Absorption spectrum of $[Ru(bpy)_2(Mes\text{-}dab)](PF_6)_2$ in acetonitrile solution.

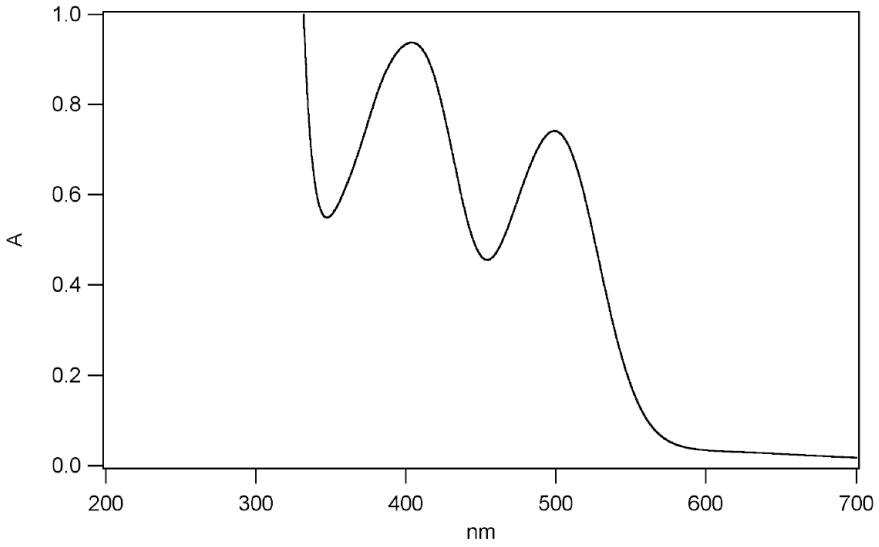

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Figure S3. Spin density for the redox states of $[Ru(bpy)_2(Mes\text{-}dab)]^{2+}$ (top) and $[Ru(bpy)_2(pyrim)]^{2+}$ (bottom).

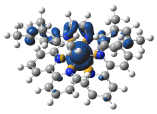
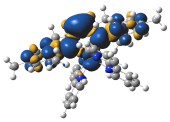
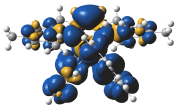
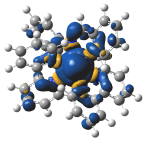
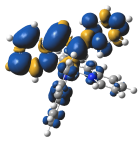
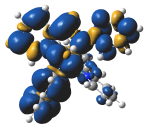
LL'= Mes-dab			
LL'=pyrim			
	$[Ru(bpy)_2(LL')]^{3+}$	$[Ru(bpy)_2(LL')]^{+}$	$[Ru(bpy)_2(LL')]^{0}$

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Figure S4. NTOs isodensity surface for main transitions of $[Ru(bpy)_2(Mes\text{-}dab)]^{2+}$

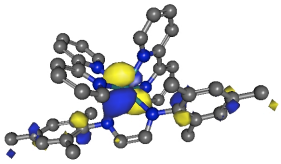
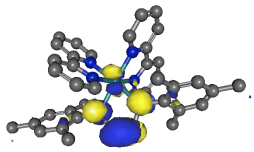
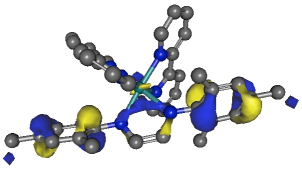
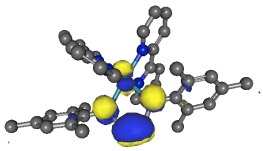
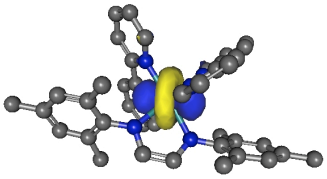
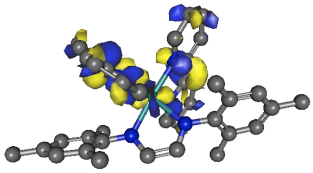
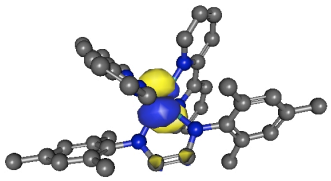
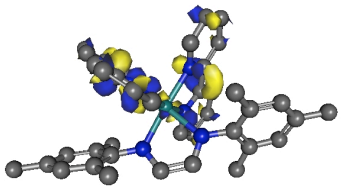
473 nm		
457 nm		
405 nm		
		
	occupied	virtual

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Table S1. Ground-state optimized Cartesian coordinates $[Ru(bpy)_2(Mes\text{-}dab)]^{2+}$ in vacuo. Molecular orbitals, eigenvalues in vacuo and in CH_3CN (in bold).

Ru	0.000000	0.000000	0.126956
N	-0.715856	1.134329	-1.549419
C	-0.404941	0.592132	-2.689732
N	2.012744	0.627420	0.293070
N	-0.738831	1.221231	1.668462
N	0.715856	-1.134329	-1.549419
N	-2.012744	-0.627420	0.293070
N	0.738831	-1.221231	1.668462
C	0.404941	-0.592132	-2.689732
C	2.760082	-0.027949	1.220910
C	2.603664	1.579979	-0.446932
C	-2.045267	1.050713	1.997523
C	-0.007821	2.091894	2.384823
C	-2.760082	0.027949	1.220910
C	-2.603664	-1.579979	-0.446932
C	2.045267	-1.050713	1.997523
C	0.007821	-2.091894	2.384823
C	4.101989	0.289307	1.419192
C	3.929365	1.945973	-0.288815
H	1.981327	2.060714	-1.189101
C	-2.632625	1.785812	3.025016
C	-0.532664	2.844843	3.420304
C	1.035158	2.185316	2.110247
C	-4.101989	-0.289307	1.419192
C	-3.929365	-1.945973	-0.288815
H	-1.981327	-2.060714	-1.189101
C	2.632625	-1.785812	3.025016
C	0.532664	-2.844843	3.420304
H	-1.035158	-2.185316	2.110247
C	4.694434	1.289015	0.664440
H	4.685249	-0.241589	2.161668
H	4.347778	2.729415	-0.912250
C	-1.874744	2.696540	3.742098
H	-3.677976	1.643936	3.271022
H	0.107827	3.534448	3.960367
C	-4.694434	-1.289015	0.664440
H	-4.685249	0.241589	2.161668
H	-4.347778	-2.729415	-0.912250
C	1.874744	-2.696540	3.742098
H	3.677976	-1.643936	3.271022
H	-0.107827	-3.534448	3.960367
H	5.738080	1.546924	0.816947
H	-2.323152	3.273897	4.544795
H	-5.738080	-1.546924	0.816947
H	2.323152	-3.273897	4.544795
H	-0.747011	1.014096	-3.632700
H	0.747011	-1.014096	-3.632700
C	1.697116	-2.194963	-1.573688
C	1.390139	-3.454766	-1.012997
C	2.965524	-1.973912	-2.157085
C	2.372762	-4.434795	-0.982307
C	3.916504	-2.993730	-2.076807
C	3.654482	-4.226035	-1.492806
H	2.120620	-5.407698	-0.566095
H	4.899485	-2.812426	-2.505528
C	-1.697116	2.194963	-1.573688
C	-1.390139	3.454766	-1.012997
C	-2.965524	1.973912	-2.157085
C	-3.916504	2.993730	-2.076807
C	-3.654482	4.226035	-1.492806
H	-2.120620	5.407698	-0.566095
H	-4.899485	2.812426	-2.505528
C	-4.689499	5.314332	-1.450184
H	-4.429973	6.124298	-2.143324
H	-5.678995	4.944787	-1.730268
H	-4.760135	5.760855	-0.452277
C	4.689499	-5.314332	-1.450184
H	4.429973	-6.124298	-2.143324
H	5.678995	-4.944787	-1.730268
H	4.760135	-5.760855	-0.452277
C	-3.383876	0.723814	-2.894881
H	-2.807617	-0.163655	-2.636218
H	-4.437653	0.505175	-2.702640
C	3.383876	-0.723814	-2.894881
H	3.287681	-0.865266	-3.978660
H	2.807617	0.163655	-2.636218
H	4.437653	-0.505175	-2.702640
C	0.000000	3.827761	-0.582942
H	0.470902	3.057629	0.024795
H	0.640590	3.996555	-1.458648
H	0.007969	4.758155	-0.010713
C	0.000000	-3.827761	-0.582942
H	-0.470902	-3.057629	0.024795
H	-0.640590	-3.996555	-1.458648
H	0.007969	-4.758155	-0.010713

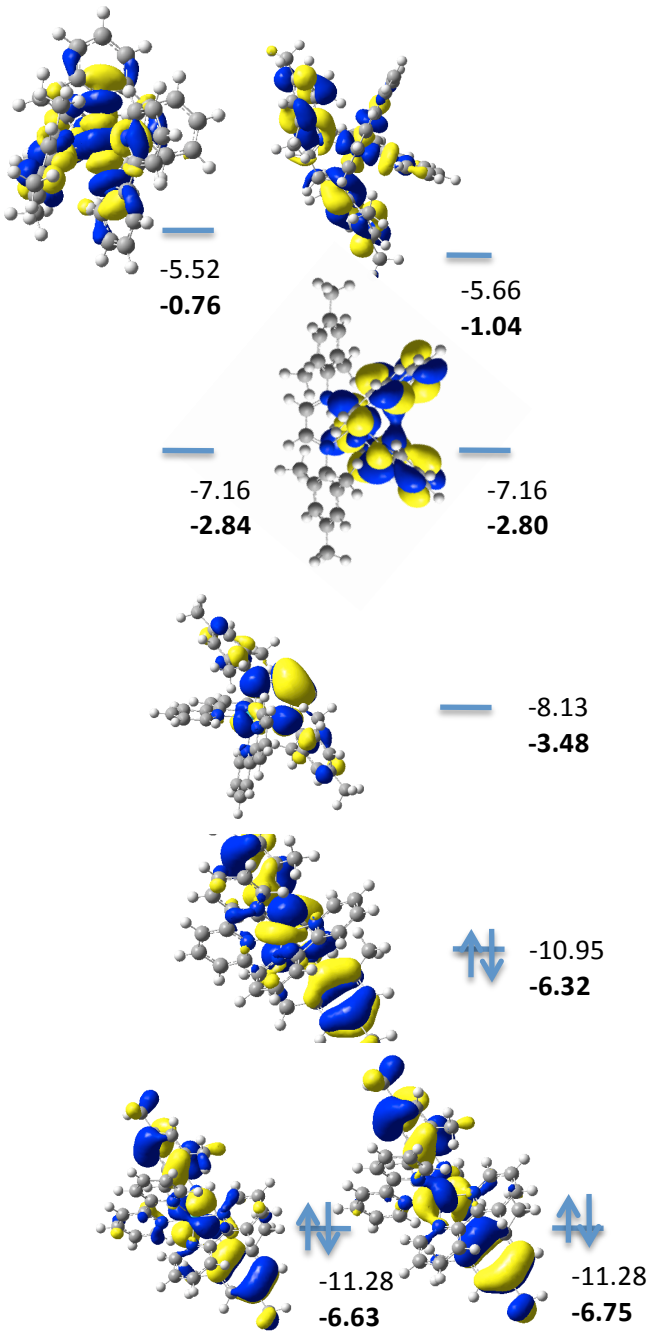

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Table S2. Optimized Cartesian coordinates and electronic structure of the ^{3}MLCT state of $[Ru(bpy)_2(Mes\text{-}dab)]^{2+}$.

Ru	0.00000000	0.00000000	0.09714980
N	-0.66413604	1.17105653	-1.50309902
C	-0.34815844	0.59233391	-2.69361061
N	2.00583792	0.64471216	0.20527339
N	-0.80382482	1.18275730	1.68174162
N	0.66413604	-1.17105653	-1.50309902
N	-2.00583792	-0.64471216	0.20527339
N	0.80382482	-1.18275730	1.68174162
C	0.34815844	-0.59233391	-2.69361061
C	2.79133845	0.01938118	1.12247036
C	2.54556868	1.59599929	-0.57311501
C	-2.12220945	1.00160938	1.94192982
C	-0.10259157	2.03741718	2.44230468
C	-2.79133845	-0.01938118	1.12247036
C	-2.54556868	-1.59599929	-0.57311501
C	2.12220945	-1.00160938	1.94192982
C	0.10259157	-2.03741718	2.44230468
C	4.13055890	0.36888179	1.27138846
C	3.86614049	1.99514272	-0.45781620
H	1.88524394	2.04170355	-1.30440379
C	-2.75813112	1.71958193	2.95192160
C	-0.67634854	2.77532271	3.46269960
H	0.95284210	2.13217399	2.21644496
C	-4.13055890	-0.36888179	1.27138846
C	-3.86614049	-1.99514272	-0.45781620
H	-1.88524394	-2.04170355	-1.30440379
C	2.75813112	-1.71958193	2.95192160
C	0.67634854	-2.77532271	3.46269960
H	-0.95284210	-2.13217399	2.21644496
C	4.67375832	1.37026707	0.48122623
H	4.74967626	-0.13571773	2.00306318
H	4.24799939	2.77691639	-1.10618544
C	-2.03285506	2.62062905	3.71489021
H	-3.81376352	1.57547278	3.14749953
H	-0.06489124	3.45780960	4.04377525
C	-4.67375832	-1.37026707	0.48122623
H	-4.74967626	0.13571773	2.00306318
H	-4.24799939	-2.77691639	-1.10618544
C	2.03285506	-2.62062905	3.71489021
H	3.81376352	-1.57547278	3.14749953
H	0.06489124	-3.45780960	4.04377525
H	5.71560500	1.65400767	0.59640275
H	-2.51960144	3.18743109	4.50287915
H	-5.71560500	-1.65400767	0.59640275
H	2.51960144	-3.18743109	4.50287915
H	-0.65490851	1.06369807	-3.62261222
H	0.65490851	-1.06369807	-3.62261222
C	1.66845024	-2.19567068	-1.49842607
C	1.38627915	-3.45355696	-0.91002807
C	2.93712889	-1.98351271	-2.08990082
C	2.38577843	-4.41547541	-0.84508501
C	3.90193476	-2.98822288	-1.99056750
C	3.66349202	-4.20450646	-1.36451613
H	2.14872531	-5.38097114	-0.40332254
H	4.87829931	-2.80748812	-2.43523227
C	-1.66845024	2.19567068	-1.49842607
C	-1.38627915	3.45355696	-0.91002807
C	-2.93712889	1.98351271	-2.08990082
C	-2.38577843	4.41547541	-0.84508501
C	-3.90193476	2.98822288	-1.99056750
C	-3.66349202	4.20450646	-1.36451613
H	-2.14872531	5.38097114	-0.40332254
H	-4.87829931	2.80748812	-2.43523227
C	-4.71404762	5.27678877	-1.29623422
H	-4.48555009	6.08938400	-1.99751106
H	-5.70434357	4.89165867	-1.55228073
H	-4.76767886	5.72481649	-0.29809443
C	4.71404762	-5.27678877	-1.29623422
H	4.48555009	-6.08938400	-1.99751106
H	5.70434357	-4.89165867	-1.55228073
H	4.76767886	-5.72481649	-0.29809443
C	-3.33269352	0.75514051	-2.87483732
H	-3.26300294	0.95323572	-3.95181935
H	-2.71850572	-0.12014593	-2.67486499
H	-4.37553369	0.49253507	-2.67481321
C	3.33269352	-0.75514051	-2.87483732
H	3.26300294	-0.95323572	-3.95181935
H	2.71850572	0.12014593	-2.67486499
H	4.37553369	-0.49253507	-2.67481321
C	0.00000000	3.85802861	-0.48679973
H	0.49238902	3.12787561	0.15396081
H	0.64025900	4.00618573	-1.36585896
H	-0.02526962	4.80864854	0.05090016
C	-0.00000000	-3.85802861	-0.48679973
H	-0.49238902	-3.12787561	0.15396081
H	-0.64025900	-4.00618573	-1.36585896
H	0.02526962	-4.80864854	0.05090016

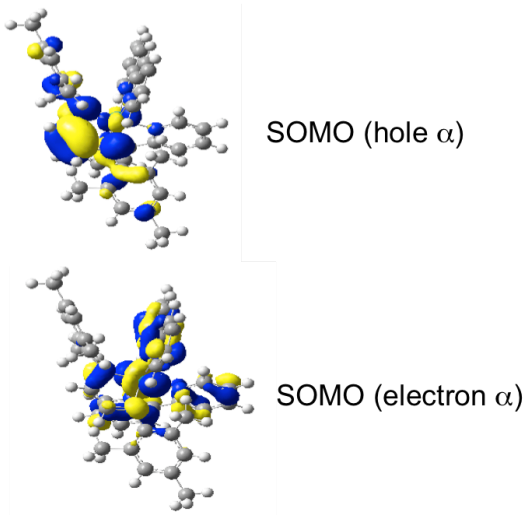

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Table S3. Optimized Cartesian coordinates and electronic structure of the ^{3}MC state of $[Ru(bpy)_2(Mes\text{-}dab)]^{2+}$.

Ru	0.00000000	0.00000000	0.02741444
N	-1.26676575	-0.34735989	-1.61103298
C	-0.68513209	-0.19198847	-2.76982100
N	0.22097367	2.47293300	0.44423122
N	-1.42369172	-0.34422278	1.64027278
N	1.26676575	0.34735989	-1.61103298
N	-0.22097367	-2.47293300	0.44423122
N	1.42369172	0.34422278	1.64027278
C	0.68513209	0.19198847	-2.76982100
C	1.25815747	2.74001567	1.25906153
C	-0.38422635	3.48369859	-0.18793236
C	-1.84014128	-1.58736058	1.98653594
C	-1.88325780	0.70775311	2.34105399
C	-1.25815747	-2.74001567	1.25906153
C	0.38422635	-3.48369859	-0.18793236
C	1.84014128	1.58736058	1.98653594
C	1.88325780	-0.70775311	2.34105399
C	1.72279609	4.04614082	1.43112609
C	0.00000000	4.80781882	-0.04129681
H	-1.21473629	3.22030932	-0.83557200
C	-2.74520037	-1.76566028	3.03393222
C	-2.78522982	0.59200318	3.38253895
H	-1.50461946	1.67792507	2.04368604
C	-1.72279609	-4.04614082	1.43112609
C	-0.00000000	-4.80781882	-0.04129681
H	1.21473629	-3.22030932	-0.83557200
C	2.74520037	1.76566028	3.03393222
C	2.78522982	-0.59200318	3.38253895
H	1.50461946	-1.67792507	2.04368604
C	1.08389245	5.08927284	0.77886092
H	2.57643151	4.25677566	2.06343274
H	-0.53495786	5.59293811	-0.56599443
C	-3.23042328	-0.67414958	3.73338575
H	-3.05979751	-2.76200236	3.31744766
H	-3.12159767	1.48096269	3.90588638
C	-1.08389245	-5.08927284	0.77886092
H	-2.57643151	-4.25677566	2.06343274
H	0.53495786	-5.59293811	-0.56599443
C	3.23042328	0.67414958	3.73338575
H	3.05979751	2.76200236	3.31744766
H	3.12159767	-1.48096269	3.90588638
H	1.43052516	6.11005552	0.91088945
H	-3.93426915	-0.81326640	4.54851848
H	-1.43052516	-6.11005552	0.91088945
H	3.93426915	0.81326640	4.54851848
H	-1.22409663	-0.34930607	-3.70176962
H	1.22409663	0.34930607	-3.70176962
C	-2.62188327	-0.84471139	-1.60972527
C	-3.64985480	-0.03360937	-1.08934866
C	-2.90869148	-2.11740182	-2.14010347
C	-4.94199213	-0.54068086	-1.04994003
C	-4.22386298	-2.57843235	-2.05814985
C	-5.25464828	-1.81897254	-1.51597752
H	-5.73780414	0.09298453	-0.66434919
H	-4.44668350	-3.56918792	-2.44778401
C	2.62188327	0.84471139	-1.60972527
C	3.64985480	0.03360937	-1.08934866
C	2.90869148	2.11740182	-2.14010347
C	4.94199213	0.54068086	-1.04994003
C	4.22386298	2.57843235	-2.05814985
C	5.25464828	1.81897254	-1.51597752
H	5.73780414	-0.09298453	-0.66434919
H	4.44668350	3.56918792	-2.44778401
C	-6.66746501	-2.33009747	-1.47410568
H	-7.27936134	-1.84090528	-2.24253599
H	-6.71499280	-3.40709035	-1.65371668
H	-7.14195570	-2.12157923	-0.50933561
C	6.66746501	2.33009747	-1.47410568
H	7.27936134	1.84090528	-2.24253599
H	6.71499280	3.40709035	-1.65371668
H	7.14195570	2.12157923	-0.50933561
C	-1.89458564	-3.00464146	-2.81986662
H	-2.11688688	-4.05691260	-2.62501624
H	-1.93250038	-2.87512472	-3.90884494
H	-0.86701849	-2.81660864	-2.50672139
C	1.89458564	3.00464146	-2.81986662
H	2.11688688	4.05691260	-2.62501624
H	1.93250038	2.87512472	-3.90884494
H	0.86701849	2.81660864	-2.50672139
C	3.41594702	-1.40399672	-0.71627690
H	2.48885258	-1.55107701	-0.16045519
H	3.35591604	-2.02796418	-1.61797603
H	4.23893640	-1.79105747	-0.11091156
C	-3.41594702	1.40399672	-0.71627690
H	-2.48885258	1.55107701	-0.16045519
H	-3.35591604	2.02796418	-1.61797603
H	-4.23893640	1.79105747	-0.11091156

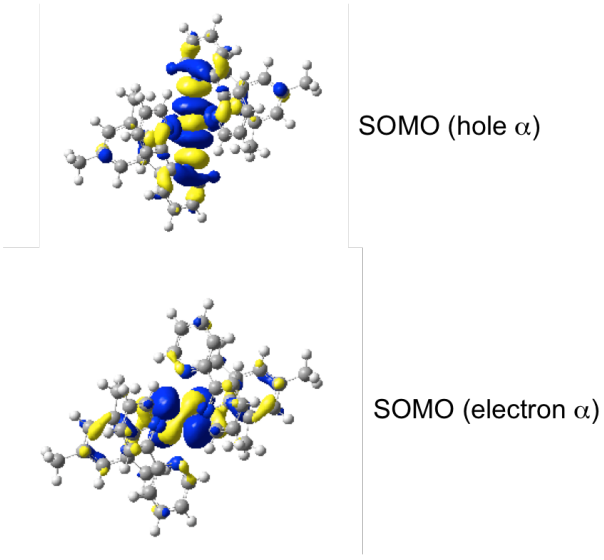

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Table S4. Ground-state optimized Cartesian coordinates of $[Ru(bpy)_2(pyrim)]^{2+}$ in vacuo. Molecular orbitals, eigenvalues in vacuo and in CH_3CN (in bold).

Ru	0.28855366	0.09760773	0.11584828
N	-0.94936324	-0.11672558	1.79419647
C	-0.96559206	0.69981831	2.86216813
H	-0.24487847	1.50900916	2.85791319
C	-1.84117227	0.53270413	3.92117574
H	-1.80831842	1.22028399	4.76008942
C	-2.74705177	-0.51931002	3.87983467
H	-3.45123278	-0.67944087	4.69062083
C	-2.73719832	-1.36677585	2.78340139
H	-3.43764308	-2.19191829	2.73469899
C	-1.82975097	-1.15191175	1.74820935
C	-1.72950601	-2.00951233	0.55634598
C	-2.50790527	-3.14779462	0.35828975
H	-3.25017574	-3.43831726	1.09211333
C	-2.32714798	-3.91744442	-0.77945012
H	-2.92800137	-4.80703273	-0.94177639
C	-1.36182916	-3.53184929	-1.69982483
H	-1.17790372	-4.10530233	-2.60254201
C	-0.62365072	-2.38776926	-1.45176083
H	0.13477004	-2.05480288	-2.15029022
N	-0.79719236	-1.63002029	-0.35654773
N	1.83638566	-1.14628012	0.78187101
C	1.89835213	-1.73785742	1.98754515
H	1.08468675	-1.52195453	2.66963101
C	2.93399360	-2.57783924	2.35900331
H	2.93335041	-3.02743842	3.34665944
C	3.95290962	-2.82754973	1.44887824
H	4.77926166	-3.48379845	1.70443157
C	3.89789434	-2.22308520	0.20301426
H	4.68354292	-2.40800893	-0.51994801
C	2.83186086	-1.38363770	-0.11434428
C	2.69483058	-0.68830284	-1.40485375
C	3.63408909	-0.76992196	-2.43089273
H	4.52511836	-1.37471186	-2.31090329
C	3.43156429	-0.06906357	-3.60933347
H	4.15848321	-0.12639306	-4.41378202
C	2.28801016	0.70852156	-3.73678075
H	2.08813800	1.27979575	-4.63755083
C	1.38885619	0.75082869	-2.68496919
H	0.48863021	1.35046266	-2.74598651
N	1.57123594	0.06656586	-1.54175722
N	1.18714181	1.91435355	0.67489593
C	2.36030324	2.09256432	1.29994765
H	2.90347515	1.19524025	1.57410446
C	2.86957437	3.35096007	1.59269941
H	3.82452605	3.43401732	2.10184813
C	2.14796434	4.48061800	1.22703983
H	2.52539167	5.47540319	1.44316924
C	0.93294632	4.31095154	0.57900820
H	0.33537994	5.16516272	0.27465328
C	0.47746232	3.02168665	0.31562993
C	-0.77757734	2.74751204	-0.34851686
H	-1.42565856	3.57159851	-0.64482077
N	-1.09825379	1.51624958	-0.58707583
C	-2.38936209	1.26319726	-1.15847635
C	-3.53051395	1.83733787	-0.59220434
H	-3.44879321	2.44190931	0.30669769
C	-4.77543656	1.60952226	-1.16582146
H	-5.66074874	2.05305553	-0.71956679
C	-4.88778185	0.82036596	-2.30489560
H	-5.86066714	0.65191028	-2.75676879
C	-3.74972737	0.24613098	-2.86426937
H	-3.83312517	-0.36175411	-3.76048191
C	-2.50355875	0.45289967	-2.28821308
H	-1.61874119	0.01331947	-2.73411970

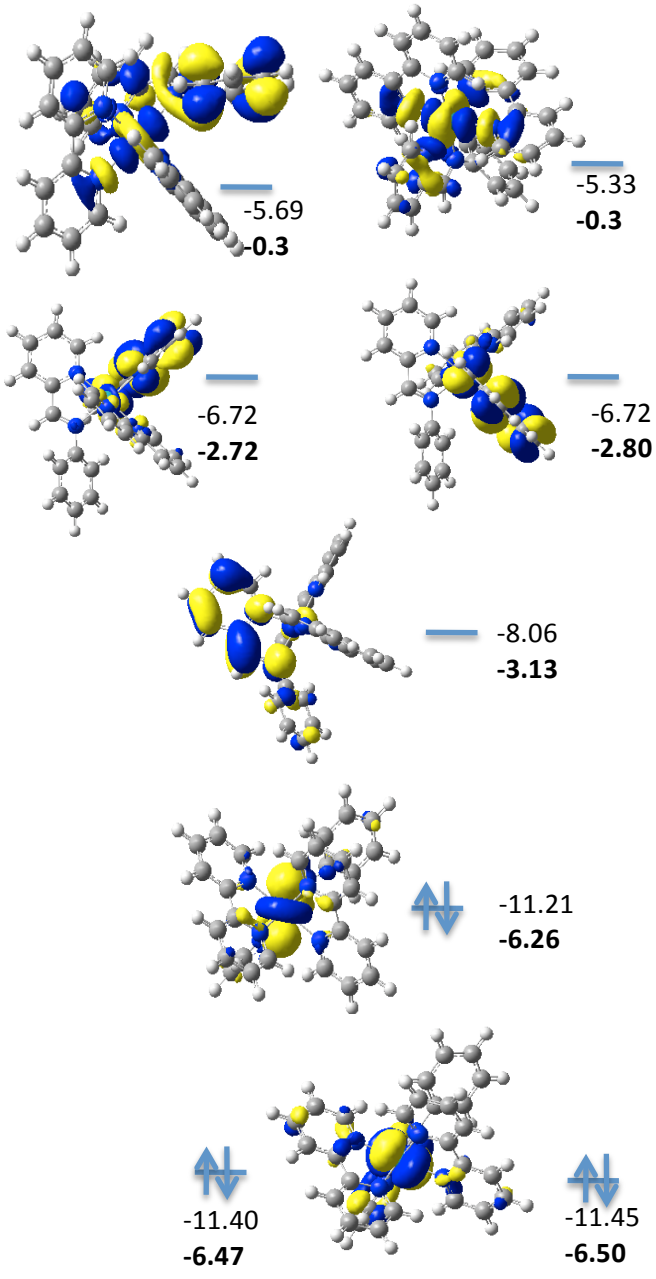

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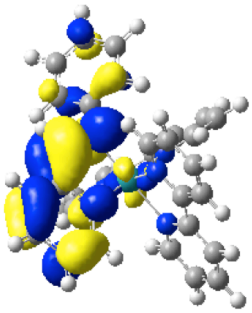
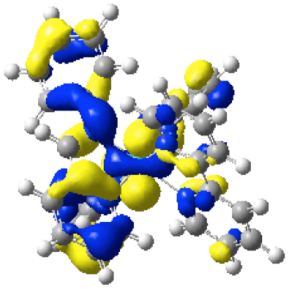
Table S5. Optimized Cartesian coordinates and electronic structure of the ^{3}MLCT state of $[Ru(bpy)_2(pyrim)]^{2+}$.

Ru	0.27649762	0.08820715	0.08921407
N	-1.07071361	-0.01154496	1.68285612
C	-1.12926863	0.87714814	2.69014967
H	-0.38694891	1.66616778	2.67711756
C	-2.08069484	0.79870551	3.69148644
H	-2.08631322	1.53724149	4.48646469
C	-3.01495822	-0.22849732	3.64713448
H	-3.77973189	-0.31552094	4.41323567
C	-2.96127410	-1.14469917	2.60807643
H	-3.68698393	-1.94763398	2.55926095
C	-1.97799595	-1.02349818	1.62989046
C	-1.82491733	-1.95368219	0.49973296
C	-2.62276361	-3.07943001	0.31127061
H	-3.42540985	-3.30634973	1.00273930
C	-2.38485997	-3.91653102	-0.76745577
H	-3.00226571	-4.79580711	-0.92475652
C	-1.34483062	-3.61430094	-1.63643288
H	-1.11904057	-4.24330322	-2.49134372
C	-0.58887074	-2.47925728	-1.39928741
H	0.22515310	-2.20379628	-2.06025047
N	-0.82066996	-1.65870709	-0.36394113
N	1.78242779	-1.22004675	0.85254415
C	1.74700319	-1.83573587	2.04512556
H	0.87813957	-1.64053735	2.66364163
C	2.75966131	-2.67215379	2.48249638
H	2.68750969	-3.14234746	3.45779146
C	3.85055437	-2.88893206	1.65062209
H	4.66291120	-3.54011153	1.95933109
C	3.88978546	-2.26172753	0.41464008
H	4.73346322	-2.42488712	-0.24536361
C	2.84357382	-1.42606029	0.03030422
C	2.79465729	-0.71462611	-1.25961143
C	3.80263338	-0.77753415	-2.21790142
H	4.68880554	-1.37632064	-2.04422975
C	3.67395874	-0.06347564	-3.40005894
H	4.45610709	-0.10580233	-4.15214065
C	2.53614143	0.70564313	-3.60165042
H	2.39503159	1.28368869	-4.50913892
C	1.56451860	0.73368693	-2.61519564
H	0.66098642	1.32207358	-2.72277031
N	1.68280911	0.03736199	-1.47218157
N	1.21717947	1.84716412	0.67467969
C	2.37503846	1.99731554	1.34478329
H	2.86484510	1.08718682	1.67417215
C	2.92138500	3.23072199	1.62788661
H	3.85008618	3.29149256	2.18437569
C	2.25242532	4.39402199	1.18960856
H	2.66574143	5.37459349	1.40501319
C	1.08276658	4.27231417	0.49155572
H	0.54434234	5.14556449	0.13608547
C	0.55274497	2.98165581	0.21778215
C	-0.60825545	2.74208003	-0.50444603
H	-1.21318704	3.55876187	-0.88599505
N	-0.98601477	1.44209575	-0.76078388
C	-2.30545059	1.22788552	-1.23243075
C	-3.39151478	1.93046276	-0.68941343
H	-3.23148329	2.62928550	0.12681986
C	-4.67360589	1.72855944	-1.18243350
H	-5.50571748	2.27998894	-0.75384664
C	-4.89522926	0.82990001	-2.22155189
H	-5.89754592	0.68374274	-2.61262181
C	-3.82129078	0.13297805	-2.76850387
H	-3.98372100	-0.54926308	-3.59818643
C	-2.53710073	0.32751216	-2.27991666
H	-1.69959377	-0.18618095	-2.74057171



SOMO (hole α)



SOMO (electron α)

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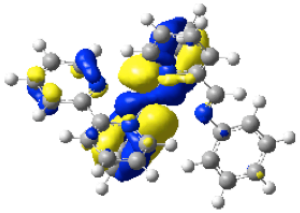
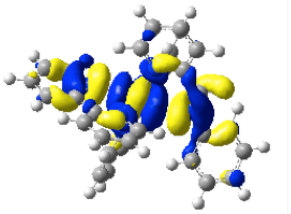
Table S6. Optimized Cartesian coordinates and electronic structure of the ^{3}MC state of $[Ru(bpy)_2(pyrim)]^{2+}$.

Ru	0.26533953	0.05894786	0.19424204
N	-0.96861645	-0.67253789	1.72347096
C	-1.25862633	-0.02323509	2.86590698
H	-0.82531057	0.96345937	2.98028324
C	-2.06048550	-0.56633985	3.85304744
H	-2.25891819	-0.00046972	4.75745892
C	-2.59684498	-1.83329091	3.65742645
H	-3.23310443	-2.28936402	4.40982966
C	-2.30494150	-2.51049836	2.48478216
H	-2.71294610	-3.50041896	2.31869358
C	-1.48540072	-1.91705270	1.52691568
C	-1.10610798	-2.56055696	0.26409573
C	-1.55862669	-3.81681087	-0.13371631
H	-2.23880816	-4.37868657	0.49525316
C	-1.13921652	-4.34900549	-1.34189600
H	-1.48825217	-5.32658812	-1.66045668
C	-0.26712209	-3.61269581	-2.13461352
H	0.08889287	-3.99076264	-3.08741250
C	0.15025419	-2.37191023	-1.68899427
H	0.83108262	-1.76761270	-2.27698894
N	-0.25469461	-1.84445570	-0.51982270
N	2.46609802	-0.86487932	0.68076211
C	2.79853505	-1.67064003	1.69378514
H	2.06202970	-1.77835912	2.48651631
C	4.01178098	-2.33976978	1.75471612
H	4.24353692	-2.97729421	2.60195018
C	4.90720766	-2.17328435	0.70591019
H	5.86380066	-2.68754975	0.70755777
C	4.56443198	-1.34371889	-0.35183923
H	5.25297284	-1.22195984	-1.17958878
C	3.33069775	-0.68931311	-0.33621499
C	2.89018901	0.22411758	-1.41926720
C	3.75662715	0.65987831	-2.42266695
H	4.79350960	0.34646910	-2.42071133
C	3.30067190	1.50801111	-3.41858830
H	3.97412963	1.84812285	-4.19961276
C	1.97430391	1.91754303	-3.39350927
H	1.56848648	2.58104759	-4.15018201
C	1.16330520	1.46643797	-2.36771913
H	0.12399602	1.76991504	-2.30316068
N	1.59639102	0.63744604	-1.39993793
N	0.58211028	2.03583954	0.97844108
C	1.72554975	2.37986107	1.59279781
H	2.47186271	1.59811151	1.68551320
C	1.95872057	3.65107656	2.09724009
H	2.90086167	3.86619296	2.59110823
C	0.97436554	4.62088538	1.96080680
H	1.12492858	5.62567233	2.34401981
C	-0.20788911	4.27856654	1.32183048
H	-1.00142345	5.00831579	1.18986932
C	-0.38244369	2.98399060	0.83403384
C	-1.61804115	2.61681718	0.14809375
H	-2.41432587	3.36740945	0.14269093
N	-1.74087628	1.48203371	-0.43185245
C	-2.96100187	1.09885554	-1.03395193
C	-4.20843806	1.48592865	-0.52602059
H	-4.27367499	2.07223947	0.38616014
C	-5.37108573	1.08764653	-1.16948982
H	-6.33571331	1.38436068	-0.76799097
C	-5.30605895	0.30717447	-2.32074784
H	-6.21949879	0.00411968	-2.82374614
C	-4.06937112	-0.09307959	-2.81834757
H	-4.01675992	-0.70198107	-3.71619703
C	-2.90220081	0.28456898	-2.17004582
H	-1.93560491	-0.02316441	-2.55749347



SOMO (hole α)



SOMO (electron α)