Conventional and cyclometalated Ir^{III}-based DNA intercalators that are isostructural with $[Ru^{II}(NN)_2(dppz)]$ light-switch systems
Supplementary information

Sasha Stimpson,[1] Dan Jenkinson,[1] Andrew Sadler,[1] Anthony J. H. M. Meijer,[1] and Jim A. Thomas[1,*]

[1] *Department of Chemistry, University of Sheffield, Brook Hill, Sheffield, S3 7HF, United Kingdom*

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* james.thomas@sheffield.ac.uk

CONTENTS

S1. EXPERIMENTAL DETAILS

S1.1. Synthesis of $[Ir(bpy)_2(dppz)](PF_6)_3$; $[\mathbf{1}](PF_6)_3$

To a sample of $[Ir(bpy)_2(OTf)_2](OTf)$ (0.58 g, 0.61 mmol) suspended in 2-propanol (60 mL) was added dipyrido[3,2-a:2,3-c]phenazine (0.18 g, 0.61 mmol). The mixture was heated to reflux for 72 hours. After allowing the solution to return to room temperature, it was evaporated to dryness to give a brown/green solid. Distilled water (30 mL) was added to the solid and dissolution of the majority was aided by heating and stirring. The orange solution was filtered before adding an excess of ammonium hexafluorophosphate to give instant precipitation of the product as a yellow solid, collected by vacuum filtration. (0.36 g, 0.30 mmol, 50%), δH (400 MHz, CD_3CN) 9.98 (dd, 2H) 8.75 (td, 2H) 8.70 (m, 2H) 8.57 (dd, 2H) 8.49 (dd, 2H) 8.38 (m, 2H) 8.25 (dd, 2H) 8.16 (m, 2H) 7.84 (m, 2H) 7.77 (m, 2H) 7.71 (m, 2H) 7.56 (m, 2H), TOF MS ES+; m/z (%): 1077 (7) $[M^+ - (PF_6)]$ 931 (14) $[M^+ -(PF_6)_2]$ 466 (12) $[M^{2+} - (PF_6)_2]$ 262 (51) $[M^{3+}- (PF_6)_3]$.

S1.2. Synthesis of $[Ir(phen)_2(bppz)](PF_6)_2$; $[\mathbf{2}](PF_6)_2$

To a sample of $[Ir(phen)_2(OTf)_2](OTf)$ (0.11 g, 0.12 mmol) suspended in 2-propanol (50 mL) was added benzo[a]pyrido-[2,3-c]phenazine, (0.034 g, 0.12 mmol). The mixture was heated to reflux for 72 hours. After allowing the solution return to room temperature, it was evaporated to dryness to give a brown/green solid. Distilled water (30 mL) was added to the solid and dissolution was aided by heating and stirring. The orange solution was filtered before adding an excess of ammonium hexafluorophosphate to give instant precipitation of the product as a pale brown solid, collected by vacuum filtration. The solid was redissolved in acetonitrile (3 mL) and passed through an alumina plug). 0.05 g, 0.044 mmol, 37%, δH (400 MHz, CD_3CN) 9.98 (dd, 2H) 8.75 (td, 2H) 8.70 (m, 2H) 8.57 (dd, 2H) 8.49 (dd, 2H) 8.38 (m, 2H) 8.25 (dd, 2H) 8.16 (m, 2H) 7.84 (m, 2H) 7.77 (m, 2H) 7.71 (m, 2H) 7.56 (m, 2H); TOF MS ES+; m/z (%): 393 (100) $[M^{2+}]$. Spectroscopic and DNA binding studies were performed on samples that were additionally purified through HPLC: a sample of the product was dissolved in acetonitrile and eluted through a column initially using 15% acetonitrile in water, which was increased over 20 minutes to 60% organic phase with a flow rate of 17 ml/min. The major peak, which began to elute off at 11.5 minutes as detected by UV/Vis spectroscopy was collected. Column used: reverse phase Walkers XBridgeTMPrep C18 5μm OBDTM 19x250 mm.

S2. COMPUTATIONAL DETAILS

Density functional theory (DFT) calculations were performed using Gaussian09, version D.01.[S1] Gaussian was compiled with Gaussian-supplied versions of BLAS and ATLAS.[S2] The B3LYP[S3] functional was used throughout with the GD3 correction[S4] to account for dispersion interactions, whereby it is noted that in this case this correction did not change the answers significantly compared to the bare B3LYP functional. The 6-311G** basis set[S5] was used on all C, N, and H. A Stuttgart-Dresden pseudopotential[S6] was used on Ru throughout. This computational procedure was found to give good correlation with experiment in previous work.[21,28,S7] The starting atomic coordinates of complex 1 are based on previous, similar systems.[21] All the calculations performed on these systems were done using water as the solvent via a polarizable continuum model (PCM)[S8] using the standard parameters as supplied by Gaussian. Visualization was done by Gausssum v2.5[S9] for the TD-DFT spectra, Jmol[S10] and Povray[S11] for the geometries. Finally, supporting information was created using in-house developed software based on the OpenEye toolkit.[S12]

The following procedure was followed. First, complexes **1**, **2**, and **2'** were optimized in their singlet ground state. Harmonic frequencies were calculated upon convergence. No imaginary frequencies were found, confirming the structure as a minimum. From the optimized S_0 geometry a number of calculations were performed. First, a time-dependent DFT[S13] calculation was performed with 100 states included to obtain the absorption spectrum. Its absorption spectrum and a breakdown of the states is given below. For **2'** no TD-DFT calculation was performed.

From each S_0 geometry geometry optimizations for the T_1 states were performed. Again, frequencies were calculated in the harmonic approximation, which confirmed the structures as minima.

S2.1. Computational References

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S3. ADDITIONAL EXPERIMENTAL FIGURES

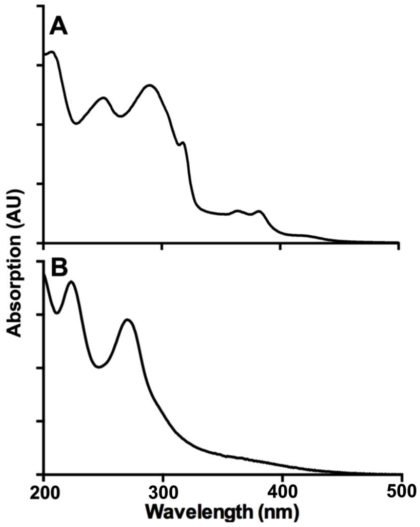


FIG. S1. Measured absorption spectra for **1** (panel A) and **2** (panel B).

S4. ADDITIONAL COMPUTATIONAL FIGURES

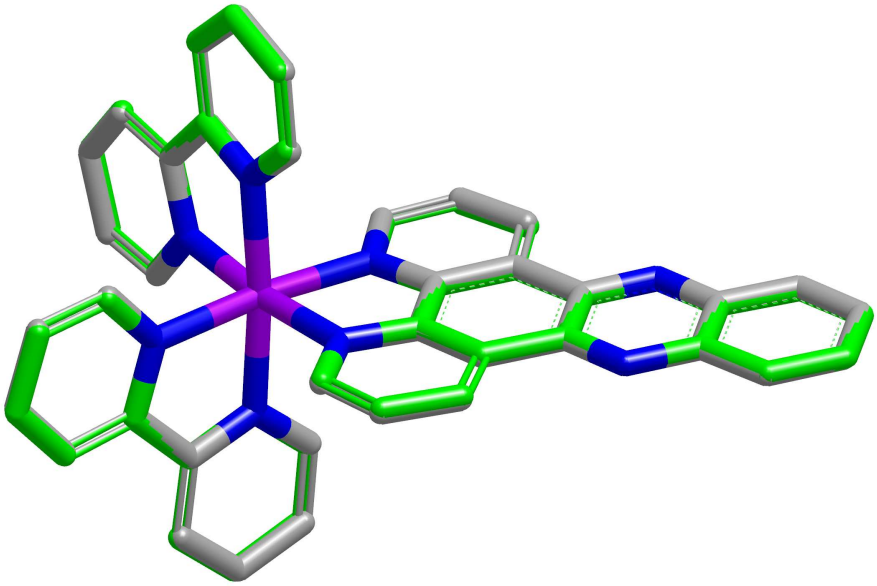


FIG. S2. Overlay between **1** (colour) and its Ru-equivalent (grey).

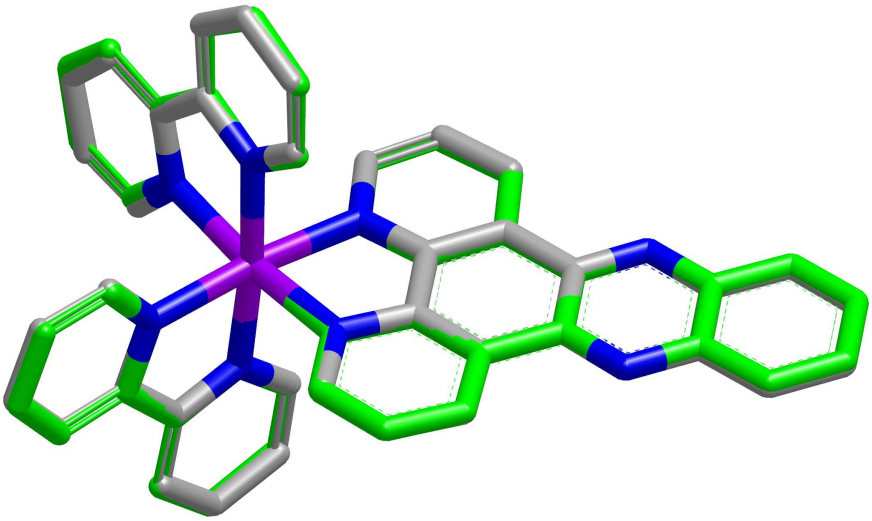


FIG. S3. Overlay between **1** (colour) and **2'** (grey) for the singlet ground state.

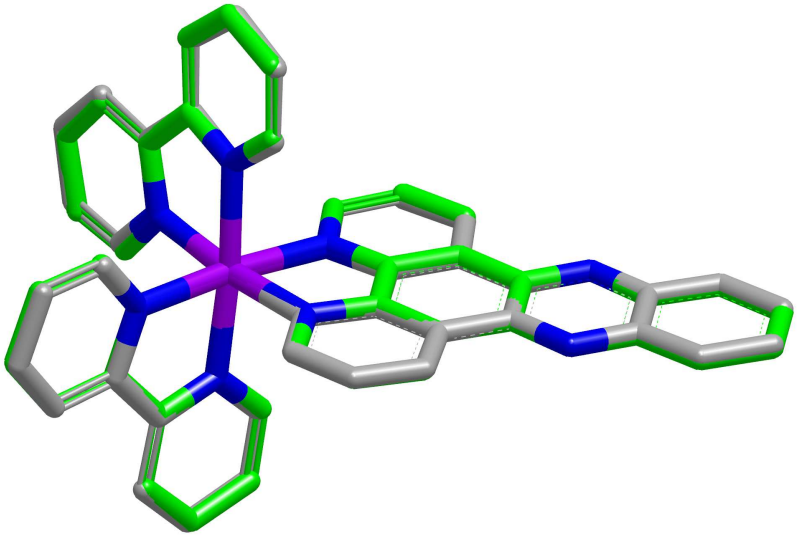


FIG. S4. Overlay between **1** (colour) and **2'** (grey) for the first triplet state.

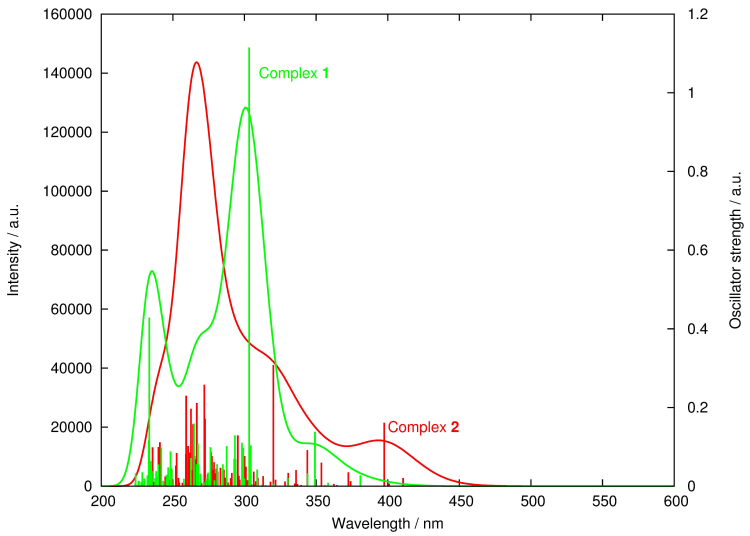
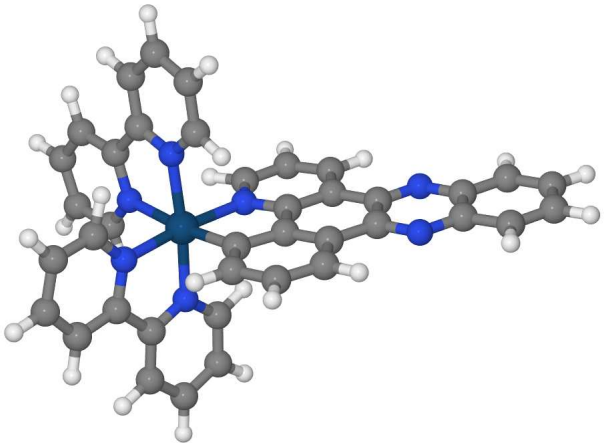


FIG. S5. Computed absorption spectra for **1** (green) and **2** (red).

S5. $[IR(BIPY)_2(BPPZ)]^{2+}$ (S_0) [2']

S5.1. General Information



SMILES	:	c1ccc2c(c1)nc-3c(n2)-c4ccc[n+]5c4-c6c3cccc6[Ir]578([n+]9 ccccc9-c1[n+]7cccc1)[n+]1ccccc1-c1[n+]8cccc1
Formula	:	$C_{39}H_{26}IrN_7^{2+}$
Charge	:	2
Multiplicity	:	1
Energy	:	-1989.90248774 a.u.
Number of imaginary frequencies	:	0

S5.2. Cartesian Co-ordinates (XYZ format)

73

N	5.34122133	-0.91749698	1.08187878
N	5.34148216	0.89353341	-1.07294965
N	0.53817242	0.81163585	-1.04736996
C	0.42618629	-1.80099404	2.06811237
H	-0.52134275	-2.14022398	2.47018814
C	1.61831057	-2.27211738	2.64359522
H	1.56642413	-2.96778274	3.47389555
C	2.85956645	-1.86535764	2.17361879
H	3.77282667	-2.23049808	2.62364721
C	2.93542910	-0.96594447	1.09994555
C	4.20666552	-0.48761761	0.55110019
C	6.50078630	-0.46284175	0.56078827
C	7.73907328	-0.89884377	1.10190368
H	7.71810722	-1.59518206	1.93139517
C	8.91750908	-0.43724385	0.57231015
C	8.91826248	0.47622573	-0.51670521
C	7.73965740	0.91736978	-1.06268215
H	7.71767902	1.61344481	-1.89240789
C	6.50252199	0.45947087	-0.53786272
C	4.21302319	0.44139761	-0.55292022
C	2.94762754	0.90705925	-1.12326860
C	2.86718416	1.80822527	-2.19122124
H	3.77856445	2.19034290	-2.63151979
C	1.62195921	2.19393969	-2.66340685

H	1.52279103	2.88846707	-3.48621297
C	0.47441679	1.67774916	-2.06765366
H	-0.51302111	1.95204306	-2.41062903
C	1.75502455	0.42396513	-0.56769562
C	1.73266542	-0.50478649	0.53130352
C	-2.12953305	-2.67052412	-0.69412893
C	-0.47388527	-2.03727627	-2.22394109
C	-2.30564213	-3.87993360	-1.36075902
C	-2.88133740	-2.26838851	0.50550747
C	-0.60998684	-3.22558141	-2.92425227
H	0.23580091	-1.28124523	-2.52510166
C	-1.54070711	-4.16123104	-2.48579025
C	-3.85932612	-3.04946494	1.11496747
H	0.00837372	-3.40353584	-3.79325032
H	-1.67098641	-5.09925222	-3.00968027
C	-3.18180871	-0.59144729	2.10980320
C	-4.50592756	-2.57741475	2.25023937
C	-4.16175365	-1.32849586	2.75597119
H	-2.87816834	0.38028413	2.47009230
H	-5.26633835	-3.17880130	2.73118067
H	-4.63733768	-0.92170089	3.63777447
N	-2.55671668	-1.04761386	1.01190138
N	-1.21775949	-1.76288795	-1.13921952
C	-2.87664652	2.32144856	-0.48221609
C	-3.31837416	0.71066636	-2.11249065
C	-3.87428784	3.14668918	-0.99851805
C	-2.04000735	2.67447472	0.68377811
C	-4.31974125	1.48869240	-2.67604637
H	-3.06068516	-0.25941762	-2.51584983
C	-4.60129166	2.72562671	-2.10585356
C	-2.12642288	3.89643788	1.34668708
H	-4.86198473	1.12521744	-3.53823066
H	-5.37850571	3.35815954	-2.51510477
C	-0.34881639	1.98147893	2.14929843
C	-1.30225503	4.15349483	2.43479300
C	-0.39916918	3.17943597	2.84383321
H	0.33457145	1.19297016	2.42796803
H	-1.36597395	5.10213757	2.95194316
H	0.26306051	3.33380890	3.68458319
N	-2.61694384	1.11596727	-1.04489934
N	-1.14827001	1.72975767	1.09680402
H	9.86384010	0.82413983	-0.91509944
H	9.86289883	-0.76927447	0.98463178
Ir	-1.07768214	-0.03211710	-0.01822689
C	0.46147749	-0.90597171	1.00356030
H	-4.08962297	4.10374403	-0.54654449
H	-2.82834864	4.64702034	1.01523793
H	-4.11444998	-4.01770020	0.71012855
H	-3.03105593	-4.59785128	-1.00704479

S5.3. Frontier Orbitals

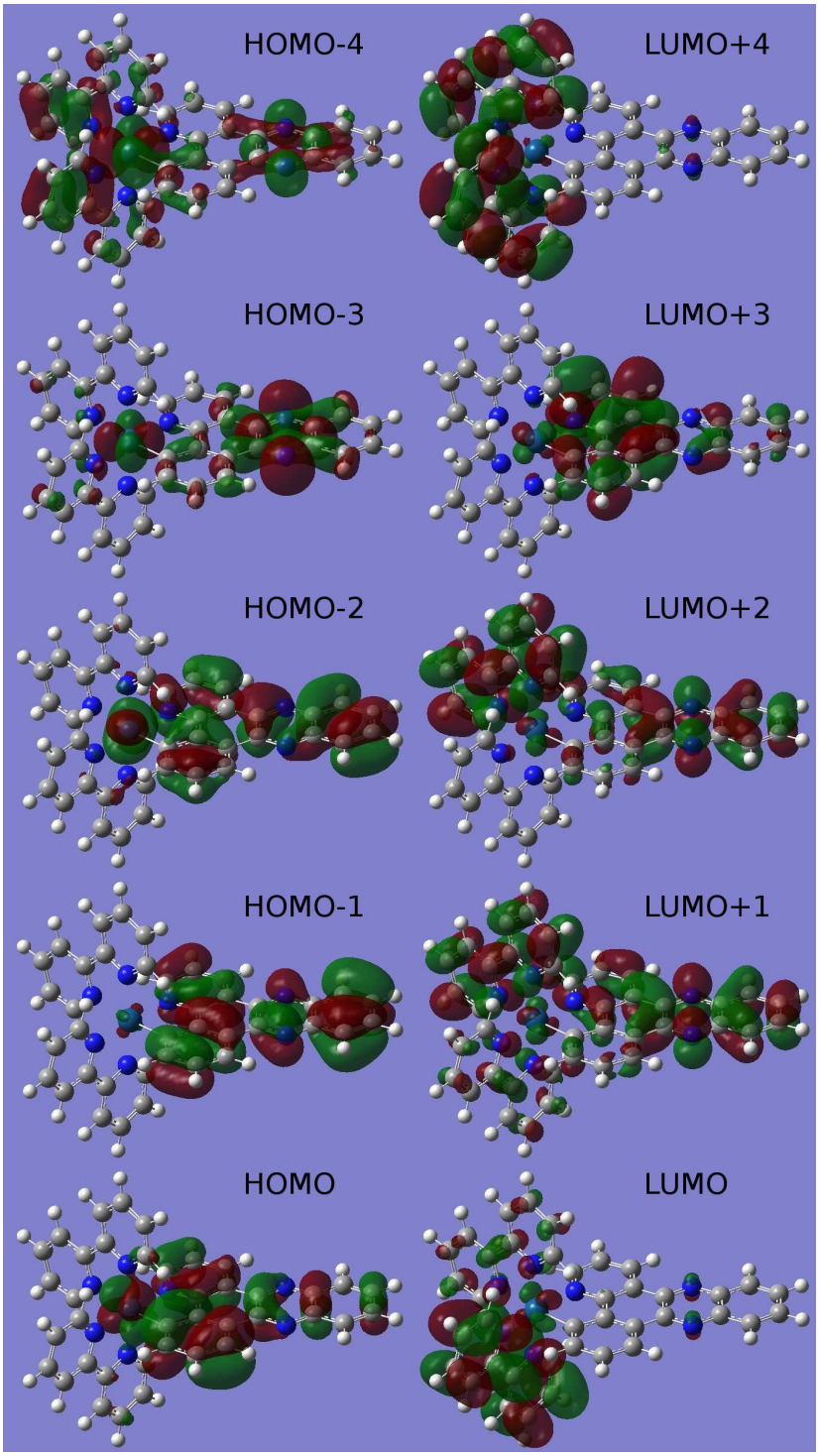
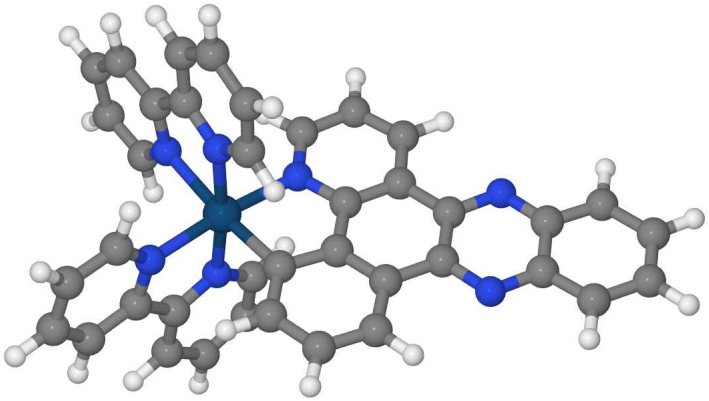


FIG. S6. Frontier orbitals for **2'**

S6. $[IR(BIPY)_2(BPPZ)]^{2+}$ (T_1) [2']

S6.1. General Information



SMILES	:	c1ccc2c(c1)nc-3c(n2)-c4ccc[n+]5c4-c6c3cccc6[Ir]578([n+]9 ccccc9-c1[n+]7cccc1)[n+]1ccccc1-c1[n+]8cccc1
Formula	:	$C_{39}H_{26}IrN_7^{2+,3}$
Charge	:	2
Multiplicity	:	3
Energy	:	-1989.81896299 a.u.
Number of imaginary frequencies	:	0

S6.2. Cartesian Co-ordinates (XYZ format)

73

N	4.27703953	-1.00175250	1.02526224
N	4.27320671	1.02962649	-0.99100012
N	-0.55797696	0.90709293	-0.97452199
C	-0.64695001	-1.97643661	1.89310682
H	-1.58740544	-2.36348367	2.26792049
C	0.56096107	-2.48744178	2.42349863
H	0.51394773	-3.25547218	3.18786550
C	1.79269326	-2.03361559	1.99500322
H	2.71002197	-2.42890000	2.40842652
C	1.86255872	-1.03229940	0.99876267
C	3.10349751	-0.49929041	0.49808195
C	5.41961813	-0.48486242	0.54036313
C	6.65809393	-0.95155805	1.03519893
H	6.64094639	-1.71988833	1.79882050
C	7.89925098	-0.43486032	0.55196488
C	7.90007067	0.53374052	-0.41188142
C	6.65689325	1.02743435	-0.93311924
H	6.65105104	1.79568172	-1.69697809
C	5.42326450	0.53849727	-0.47655752
C	3.11089253	0.50083441	-0.49266490
C	1.86728382	1.00795853	-1.02075016
C	1.78439713	2.00750208	-2.01044226
H	2.69636989	2.43000293	-2.40988350
C	0.54450893	2.42758942	-2.44976330

H	0.44663167	3.19291568	-3.20767117
C	-0.61477196	1.85757339	-1.90969586
H	-1.59847939	2.16377926	-2.23630619
C	0.65923458	0.47758430	-0.52170575
C	0.63943082	-0.53498799	0.47734943
C	-3.19289637	-2.61575818	-0.94381553
C	-1.54027987	-1.82955134	-2.40465713
C	-3.35438704	-3.76188636	-1.71743333
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C	-1.66180396	-2.95130324	-3.20965266
H	-0.83813953	-1.04166710	-2.63325667
C	-2.58354449	-3.93240523	-2.86055589
C	-4.92260599	-3.17398024	0.81845653
H	-1.03933871	-3.04380465	-4.08896208
H	-2.70232058	-4.82065058	-3.46739173
C	-4.27467585	-0.80771130	2.03154898
C	-5.57724237	-2.81239247	1.98910487
C	-5.24817181	-1.61005175	2.60571289
H	-3.98268795	0.13128728	2.47808051
H	-6.33225060	-3.46249914	2.41163373
H	-5.73064661	-1.28894186	3.51859570
N	-3.64173651	-1.15708160	0.89951414
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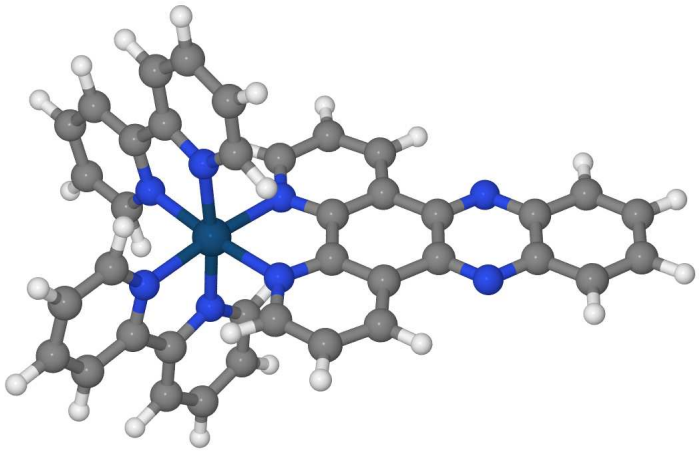
H	-6.46958876	3.54376268	-2.24163008
C	-1.46275294	1.77433968	2.31365967
C	-2.42573404	3.90946317	2.78537655
C	-1.52132165	2.90578198	3.11151338
H	-0.77832383	0.96600270	2.52488637
H	-2.49574113	4.80818462	3.38441205
H	-0.86427402	2.98710108	3.96645904
N	-3.70987844	1.18808126	-0.95708913
N	-2.25553322	1.61474299	1.23843443
H	8.82814598	0.93997592	-0.79335397
H	8.82632065	-0.81934321	0.95735508
Ir	-2.16967583	-0.03899571	-0.02963878
C	-0.62745970	-0.99232680	0.91651034
H	-5.19440079	4.11690617	-0.20737912
H	-3.94586658	4.52235889	1.40637946
H	-5.16604471	-4.10476780	0.32768130
H	-4.07289553	-4.51641321	-1.43246269

S7. $[IR(BIPY)_2(DPPZ)]^{3+}$ (S_0) [1]

S7.1. General Information



SMILES	:	c1ccc2c(c1)nc3=c4ccc[n+]5c4=c6c(=c3n2)ccc[n+]6[Ir]578([n+]9ccccc9-c1[n+]7cccc1)[n+]1ccccc1-c1[n+]8cccc1
Formula	:	$C_{38}H_{26}IrN_8^{3+}$
Charge	:	3
Multiplicity	:	1
Energy	:	-2006.39685450 a.u.
Number of imaginary frequencies	:	0

S7.2. Cartesian Co-ordinates (XYZ format)

73

N	-0.54702288	-0.95576805	0.93256676
N	4.26011038	-1.01867318	0.96785778
N	4.25763226	1.01472795	-0.98244804
N	-0.54938692	0.95567036	-0.93097454
C	-0.60933632	-1.92269146	1.85415995
H	-1.59317887	-2.23528910	2.17211366
C	0.54487616	-2.49425483	2.38989711
H	0.44747674	-3.27216482	3.13432503
C	1.78605556	-2.05734515	1.96532023
H	2.69927335	-2.47805166	2.36375904
C	1.86500704	-1.04554832	0.99621254
C	3.13191628	-0.51945889	0.49082607
C	5.41757250	-0.52128613	0.48935136
C	6.65563917	-1.02334166	0.97002709
H	6.63564968	-1.80390644	1.72030854
C	7.83098459	-0.51594049	0.48008159
C	7.82972813	0.50949061	-0.50637567
C	6.65314007	1.01771641	-0.99246728
H	6.63124037	1.79831159	-1.74266398
C	5.41630459	0.51650614	-0.50775915
C	3.13065839	0.51633531	-0.50168961
C	1.86248064	1.04343474	-1.00281227
C	1.78108501	2.05526972	-1.97167921
H	2.69329429	2.47520328	-2.37323141

C	0.53883743	2.49316883	-2.39208913
H	0.43955794	3.27113509	-3.13620996
C	-0.61402261	1.92257297	-1.85242343
H	-1.59868312	2.23599577	-2.16702032
C	0.66672295	0.51973295	-0.50085741
C	0.66798663	-0.52083457	0.49833873
C	-3.17651653	-2.57595706	-0.93116975
C	-1.48140991	-1.81354249	-2.35948420
C	-3.32856655	-3.72550988	-1.69946682
C	-3.96157980	-2.27991724	0.27839389
C	-1.59262192	-2.94114733	-3.15754795
H	-0.77267885	-1.03139234	-2.58669662
C	-2.53081989	-3.91053843	-2.82239676
H	-4.05928612	-4.47240353	-1.42658186
C	-4.96455622	-3.10276890	0.77979034
H	-0.95132083	-3.04457664	-4.02172422
H	-2.64313817	-4.80227900	-3.42511964
C	-4.29434824	-0.76157808	2.03370762
C	-5.64036179	-2.73444462	1.93702412
H	-5.21877003	-4.02234936	0.27415699
C	-5.29976606	-1.54715633	2.57473469
H	-3.99323606	0.16572422	2.49737644
H	-6.42181778	-3.36978984	2.33276033
H	-5.79775715	-1.22286117	3.47783828
N	-3.64163375	-1.11925781	0.91489750
N	-2.25544381	-1.63417804	-1.27595842
C	-3.96012616	2.28328085	-0.26479816
C	-4.30074787	0.76525825	-2.01886582
C	-4.96401262	3.10717916	-0.76263994
C	-3.17040682	2.57856750	0.94191295
C	-5.30726910	1.55187464	-2.55632520
H	-4.00225973	-0.16236326	-2.48358750
C	-5.64434242	2.73953319	-1.91743708
H	-5.21544600	4.02704287	-0.25613180
C	-3.31835246	3.72842360	1.71055377
H	-5.80881023	1.22808433	-3.45764375
H	-6.42652082	3.37570214	-2.31041217
C	-1.47100639	1.81445241	2.36420774
C	-2.51635885	3.91270924	2.83057666
H	-4.04915142	4.47614241	1.44015145
C	-1.57807255	2.94229484	3.16250348
H	-0.76234263	1.03153729	2.58898211
H	-2.62544584	4.80469942	3.43352342
H	-0.93354195	3.04512358	4.02434540
N	-3.64368200	1.12226188	-0.90239692
N	-2.24916005	1.63579798	1.28351796
H	8.77555084	0.88912570	-0.87345457
H	8.77773857	-0.89622051	0.84407800
Ir	-2.15089083	0.00073140	0.00362719

S7.3. TD-DFT calcuations

TABLE S4: Major transitions ($f > 0.04$) for $[Ir(bipy)_2(dppz)]^{3+}$ in water. Additionally, the transition to S_1 is included.

No.	Energy (cm^{-1})	Wavelength (nm)	Osc. strength	Major Contribs
1	24249	412.38	0.02	HOMO⟶LUMO (92%)
3	25090	398.56	0.16	HOMO⟶L+1 (93%)
6	26854	372.39	0.04	H-1⟶L+1 (90%)
10	28183	354.83	0.06	HOMO⟶L+5 (83%)

11	28970	345.18	0.09	H-3⟶LUMO (58%), H-2⟶LUMO (24%)
14	29654	337.22	0.04	H-3⟶L+2 (57%), H-2⟶L+2 (13%)
16	30160	331.57	0.04	H-6⟶L+2 (10%), H-5⟶L+2 (13%), H-3⟶L+2 (13%), H-2⟶L+2 (43%)
19	31224	320.26	0.31	H-2⟶L+1 (33%), H-1⟶L+5 (45%)
32	33279	300.49	0.07	H-7⟶LUMO (16%), H-5⟶L+3 (22%), H-4⟶L+2 (13%)
36	33792	295.92	0.14	H-7⟶L+2 (12%), H-5⟶L+3 (15%), H-2⟶L+5 (10%), HOMO⟶L+6 (20%)
38	34349	291.13	0.05	H-9⟶L+2 (20%), H-7⟶L+2 (16%), H-5⟶L+4 (21%)
44	35205	284.05	0.04	H-6⟶L+4 (25%), H-4⟶L+4 (38%)
49	35843	279.00	0.06	H-9⟶LUMO (31%), H-8⟶L+1 (10%), H-7⟶L+3 (13%), H-6⟶L+4 (13%)
50	35883	278.68	0.11	H-7⟶L+3 (26%), HOMO⟶L+9 (11%)
51	35998	277.79	0.05	H-9⟶LUMO (28%), H-8⟶L+1 (21%)
53	36144	276.67	0.06	H-8⟶L+1 (45%), H-6⟶L+4 (10%), H-6⟶L+5 (10%)
55	36703	272.46	0.09	H-10⟶L+2 (47%)
56	36775	271.92	0.38	H-9⟶L+1 (21%), H-7⟶L+1 (10%), H-1⟶L+6 (26%)
59	37369	267.60	0.07	HOMO⟶L+8 (46%)
60	37460	266.95	0.04	H-9⟶L+9 (13%), H-7⟶L+9 (10%), H-2⟶L+9 (12%), HOMO⟶L+8 (24%)
61	37516	266.55	0.22	H-9⟶L+1 (44%), H-6⟶L+5 (13%), H-1⟶L+6 (11%)
62	37596	265.98	0.09	H-10⟶L+3 (13%), H-9⟶L+3 (20%)
64	37752	264.89	0.04	H-11⟶LUMO (15%), HOMO⟶L+8 (11%)
65	37858	264.15	0.11	H-10⟶L+1 (10%), H-10⟶L+3 (11%), H-8⟶L+4 (17%)
67	38058	262.76	0.12	H-11⟶LUMO (16%), H-7⟶L+5 (21%)
69	38262	261.35	0.18	H-11⟶L+2 (18%), H-10⟶L+3 (10%), H-9⟶L+3 (14%)
70	38307	261.05	0.11	H-9⟶L+3 (24%), H-9⟶L+4 (36%)
71	38513	259.65	0.20	H-11⟶LUMO (33%), H-11⟶L+2 (17%)
72	38548	259.42	0.17	H-8⟶L+5 (15%), H-2⟶L+6 (28%)
78	39638	252.28	0.14	H-8⟶L+5 (46%), H-2⟶L+6 (19%)
91	41402	241.53	0.13	H-3⟶L+7 (26%), H-2⟶L+7 (30%)
92	41569	240.56	0.11	H-3⟶L+7 (29%), H-2⟶L+7 (38%)
97	42394	235.88	0.08	H-13⟶L+1 (17%), H-6⟶L+6 (20%), H-1⟶L+9 (14%), HOMO⟶L+10 (19%)

S7.4. Frontier Orbitals

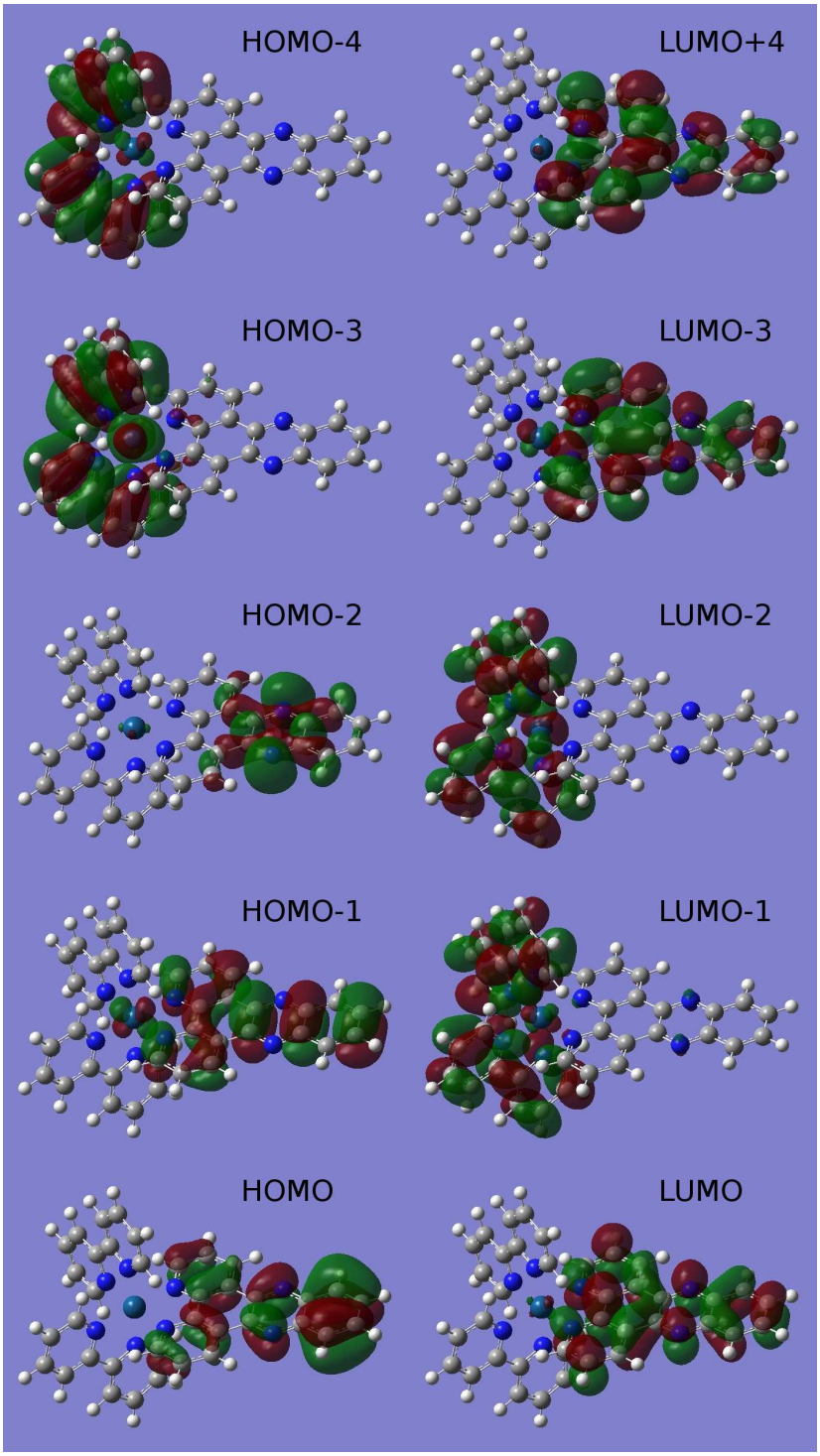
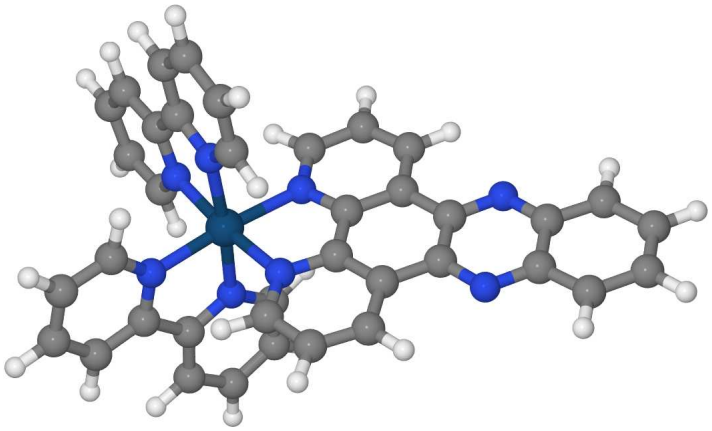


FIG. S7. Frontier orbitals for **1**

S8. $[IR(BIPY)_2(DPPZ)]^{3+}$ (T_1) [1]

S8.1. General Information



SMILES	:	c1ccc2c(c1)nc-3c(n2)-c4ccc[n+]5c4-c6c3ccc[n+]6[Ir]578([n+]9ccccc9-c1[n+]7cccc1)[n+]1ccccc1-c1[n+]8cccc1
Formula	:	$C_{38}H_{26}IrN_8^{3+,3}$
Charge	:	3
Multiplicity	:	3
Energy	:	-2006.31619090 a.u.
Number of imaginary frequencies	:	0

S8.2. Cartesian Co-ordinates (XYZ format)

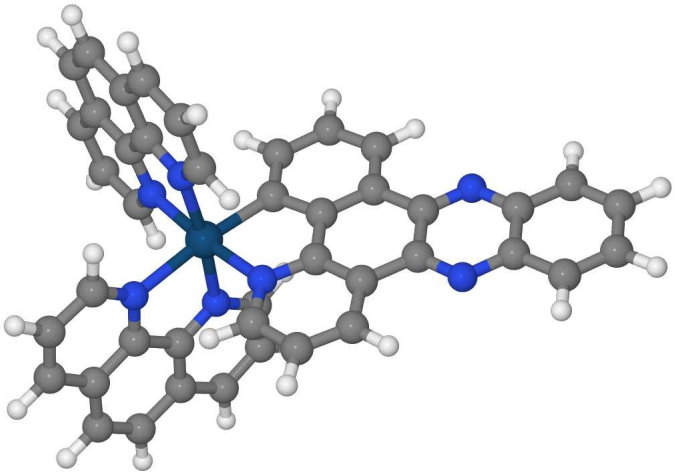
73

N	-0.56175083	-0.95753837	0.93555063
N	4.27315950	-1.03149605	0.98607403
N	4.27069998	1.02766109	-1.00043845
N	-0.56410903	0.95774257	-0.93371785
C	-0.61205477	-1.91956019	1.85546875
H	-1.59136665	-2.23987484	2.18060088
C	0.55453974	-2.48611355	2.38921666
H	0.46132469	-3.26295233	3.13539433
C	1.78847802	-2.04725599	1.96216989
H	2.70431948	-2.46355939	2.35855198
C	1.86580777	-1.03069901	0.98526025
C	3.11045146	-0.50813746	0.48226818
C	5.41487694	-0.52015883	0.49176219
C	6.65593529	-1.00515795	0.96011883
H	6.64542723	-1.78324628	1.71363699
C	7.89947987	-0.49315357	0.46178913
C	7.89830303	0.48601463	-0.48853534
C	6.65353203	0.99916023	-0.98261076
H	6.64116287	1.77725196	-1.73609698
C	5.41363573	0.51530445	-0.51000804
C	3.10924029	0.50536716	-0.49265695
C	1.86335003	1.02895916	-0.99149430
C	1.78359032	2.04562593	-1.96809411
H	2.69843888	2.46122456	-2.36749506

C	0.54858923	2.48551464	-2.39099002
H	0.45351782	3.26246738	-3.13681507
C	-0.61668301	1.91988838	-1.85338616
H	-1.59679842	2.24099422	-2.17530465
C	0.65033728	0.51220977	-0.49407625
C	0.65157413	-0.51299638	0.49183911
C	-3.18310881	-2.57744002	-0.93168414
C	-1.48868215	-1.81043696	-2.35851526
C	-3.33183146	-3.72726727	-1.70034528
C	-3.96842098	-2.28405094	0.27857825
C	-1.59632289	-2.93838954	-3.15676141
H	-0.78131020	-1.02640224	-2.58366179
C	-2.53266025	-3.90999627	-2.82271647
H	-4.06069613	-4.47622633	-1.42810309
C	-4.96887064	-3.10997987	0.78022987
H	-0.95371729	-3.04047012	-4.02014828
H	-2.64224052	-4.80190849	-3.42572236
C	-4.30383587	-0.76773846	2.03489900
C	-5.64472532	-2.74412775	1.93825233
H	-5.22101212	-4.03000927	0.27435154
C	-5.30682802	-1.55625379	2.57638884
H	-4.00461674	0.16027364	2.49855900
H	-6.42411804	-3.38183928	2.33430028
H	-5.80505610	-1.23388660	3.48006988
N	-3.65116453	-1.12294221	0.91543460
N	-2.26456189	-1.63315380	-1.27608359
C	-3.96697378	2.28733349	-0.26525566
C	-4.31072187	0.77082425	-2.01979852
C	-4.96842480	3.11418724	-0.76336503
C	-3.17691422	2.58020687	0.94204515
C	-5.31488466	1.56027544	-2.55774236
H	-4.01430559	-0.15766650	-2.48429799
C	-5.64905357	2.74872398	-1.91871190
H	-5.21771097	4.03459835	-0.25677612
C	-3.32134271	3.73058367	1.71070921
H	-5.81691933	1.23816121	-3.45940328
H	-6.42926884	3.38714957	-2.31197977
C	-1.47869384	1.81140244	2.36338401
C	-2.51802516	3.91267443	2.83022308
H	-4.05004883	4.48049021	1.44066167
C	-1.58199549	2.93983531	3.16152358
H	-0.77169865	1.02643800	2.58647609
H	-2.62421846	4.80502510	3.43318534
H	-0.93634135	3.04131603	4.02270317
N	-3.65339637	1.12568033	-0.90295064
N	-2.25843382	1.63482869	1.28361833
H	8.82411098	0.88700801	-0.87973136
H	8.82625198	-0.89501530	0.84979892
Ir	-2.16290832	0.00072964	0.00364547

S9. $[IR(PHEN)_2(BPPZ)]^{2+}$ (S_0) [2]

S9.1. General Information



SMILES	:	c1ccc2c(c1)nc-3c(n2)-c4ccc[n+]5c4-c6c3cccc6[Ir]578([n+]9cccc1c9c2[n+]7cccc2cc1)[n+]1cccc2c1c1[n+]8cccc1cc2
Formula	:	$C_{43}H_{26}IrN_7^{2+}$
Charge	:	2
Multiplicity	:	1
Energy	:	-2142.40173106 a.u.
Number of imaginary frequencies	:	0

S9.2. Cartesian Co-ordinates (XYZ format)

77

N	4.28056431	-0.96505547	1.01899111
N	4.27356815	1.00158536	-0.99482429
N	-0.52918160	0.89093655	-0.98346770
C	-0.63203472	-1.94469309	1.92780304
H	-1.57892931	-2.31971836	2.29829502
C	0.56157708	-2.45050907	2.46987653
H	0.51175165	-3.20726705	3.24504638
C	1.80171263	-2.00238919	2.03563380
H	2.71590924	-2.39570904	2.45930481
C	1.87500274	-1.02435613	1.03277493
C	3.14431334	-0.50103319	0.52179909
C	5.43838072	-0.46884131	0.53289580
C	6.67838192	-0.94037527	1.03905118
H	6.66016150	-1.69693863	1.81408596
C	7.85502195	-0.43703315	0.54460275
C	7.85210848	0.55543107	-0.47290528
C	6.67167854	1.03272855	-0.98343456
H	6.64690256	1.78873122	-1.75887442
C	5.43641520	0.53298765	-0.49365643
C	3.14693332	0.50754803	-0.51033109
C	1.87973297	1.00758243	-1.04671216
C	1.79510558	1.98280454	-2.04713893
H	2.70454240	2.40138507	-2.45729899
C	0.54803503	2.39334989	-2.49290729

H	0.44565240	3.14467478	-3.26379251
C	-0.59719688	1.82772434	-1.93902934
H	-1.58603132	2.11864424	-2.26364517
C	0.68945473	0.47829473	-0.53006238
C	0.67099458	-0.52800453	0.49798852
C	-3.18479037	-2.58297706	-0.92561704
C	-1.54512644	-1.88326120	-2.41855311
C	-3.42871642	-3.76471829	-1.65049434
C	-3.91775250	-2.30474639	0.26372620
C	-1.72932601	-3.03593183	-3.19424534
H	-0.81724012	-1.13264811	-2.69133759
C	-2.66545296	-3.97610664	-2.81773973
C	-4.89229965	-3.20958257	0.72572422
H	-1.12640738	-3.16812110	-4.08217049
H	-2.81953120	-4.87248755	-3.40584731
C	-4.28670406	-0.84326595	2.03263426
C	-5.57696247	-2.87158132	1.91184044
C	-5.27126980	-1.69162905	2.55724812
H	-4.02544737	0.08381112	2.52283001
H	-6.33409977	-3.53934503	2.30432463
H	-5.77650166	-1.40227091	3.46851683
N	-3.62611794	-1.14147139	0.91557890
N	-2.25772619	-1.65930307	-1.31574225
C	-3.93561673	2.31581330	-0.28287593
C	-4.39392948	0.92330414	-2.08104777
C	-4.90459490	3.25704265	-0.68745369
C	-3.16134214	2.54721332	0.89810306
C	-5.37913704	1.80406249	-2.55224204
H	-4.16597319	0.00325919	-2.60358429
C	-5.63471889	2.96876717	-1.86031437
C	-3.36327291	3.72133207	1.65234327
H	-5.92253160	1.55517304	-3.45358062
H	-6.38881588	3.66545105	-2.20584750
C	-1.49993145	1.79904544	2.35057163
C	-2.56892824	3.90287232	2.80363274
C	-1.64096856	2.94320369	3.14565492
H	-0.78596509	1.02558994	2.59559560
H	-2.69507217	4.79360580	3.40703440
H	-1.01502883	3.05112863	4.02085686
N	-3.69209051	1.17288971	-0.98081249
N	-2.24061179	1.60152650	1.25944221
H	8.79631233	0.93483722	-0.84493387
H	8.80176926	-0.79626983	0.93012744
Ir	-2.13861656	-0.03830698	-0.02722825
C	-0.59879202	-0.97172868	0.93400431
C	-5.09457684	4.44034481	0.09897527
C	-4.35479307	4.66266251	1.21888185
H	-5.84201717	5.15670872	-0.21925685
H	-4.50229692	5.55954981	1.80773735
C	-5.12728119	-4.40763187	-0.02751790
C	-4.42689323	-4.67327547	-1.16447783
H	-5.87842321	-5.10073662	0.33046633
H	-4.61207247	-5.58074951	-1.72576785

S9.3. TD-DFT Calculations

TABLE S7: Major transitions ($f > 0.04$) for $[Ir(phen)_2(bppz)]^{3+}$ in water.

No.	Energy (cm^{-1})	Wave length (nm)	Osc. Strength	Major contribs

1	24249	412.38	0.02	HOMO⟶LUMO (92%)
3	25090	398.56	0.16	HOMO⟶L+1 (93%)
6	26854	372.39	0.04	H-1⟶L+1 (90%)
10	28183	354.83	0.06	HOMO⟶L+5 (83%)
11	28970	345.18	0.09	H-3⟶LUMO (58%), H-2⟶LUMO (24%)
14	29654	337.22	0.04	H-3⟶L+2 (57%), H-2⟶L+2 (13%)
16	30160	331.57	0.04	H-6⟶L+2 (10%), H-5⟶L+2 (13%), H-3⟶L+2 (13%), H-2⟶L+2 (43%)
19	31224	320.26	0.31	H-2⟶L+1 (33%), H-1⟶L+5 (45%)
32	33279	300.49	0.07	H-7⟶LUMO (16%), H-5⟶L+3 (22%), H-4⟶L+2 (13%)
36	33792	295.92	0.14	H-7⟶L+2 (12%), H-5⟶L+3 (15%), H-2⟶L+5 (10%), HOMO⟶L+6 (20%)
38	34349	291.13	0.05	H-9⟶L+2 (20%), H-7⟶L+2 (16%), H-5⟶L+4 (21%)
44	35205	284.05	0.04	H-6⟶L+4 (25%), H-4⟶L+4 (38%)
49	35843	279.00	0.06	H-9⟶LUMO (31%), H-8⟶L+1 (10%), H-7⟶L+3 (13%), H-6⟶L+4 (13%)
50	35883	278.68	0.11	H-7⟶L+3 (26%), HOMO⟶L+9 (11%)
51	35998	277.79	0.05	H-9⟶LUMO (28%), H-8⟶L+1 (21%)
53	36144	276.67	0.06	H-8⟶L+1 (45%), H-6⟶L+4 (10%), H-6⟶L+5 (10%)
55	36703	272.46	0.09	H-10⟶L+2 (47%)
56	36775	271.92	0.38	H-9⟶L+1 (21%), H-7⟶L+1 (10%), H-1⟶L+6 (26%)
59	37369	267.60	0.07	HOMO⟶L+8 (46%)
60	37460	266.95	0.04	H-9⟶L+9 (13%), H-7⟶L+9 (10%), H-2⟶L+9 (12%), HOMO⟶L+8 (24%)
61	37516	266.55	0.22	H-9⟶L+1 (44%), H-6⟶L+5 (13%), H-1⟶L+6 (11%)
62	37596	265.98	0.09	H-10⟶L+3 (13%), H-9⟶L+3 (20%)
64	37752	264.89	0.04	H-11⟶LUMO (15%), HOMO⟶L+8 (11%)
65	37858	264.15	0.11	H-10⟶L+1 (10%), H-10⟶L+3 (11%), H-8⟶L+4 (17%)
67	38058	262.76	0.12	H-11⟶LUMO (16%), H-7⟶L+5 (21%)
69	38262	261.35	0.18	H-11⟶L+2 (18%), H-10⟶L+3 (10%), H-9⟶L+3 (14%)
70	38307	261.05	0.11	H-9⟶L+3 (24%), H-9⟶L+4 (36%)
71	38513	259.65	0.20	H-11⟶LUMO (33%), H-11⟶L+2 (17%)
72	38548	259.42	0.17	H-8⟶L+5 (15%), H-2⟶L+6 (28%)
78	39638	252.28	0.14	H-8⟶L+5 (46%), H-2⟶L+6 (19%)
91	41402	241.53	0.13	H-3⟶L+7 (26%), H-2⟶L+7 (30%)
92	41569	240.56	0.11	H-3⟶L+7 (29%), H-2⟶L+7 (38%)
97	42394	235.88	0.08	H-13⟶L+1 (17%), H-6⟶L+6 (20%), H-1⟶L+9 (14%), HOMO⟶L+10 (19%)

S9.4. Frontier Orbitals

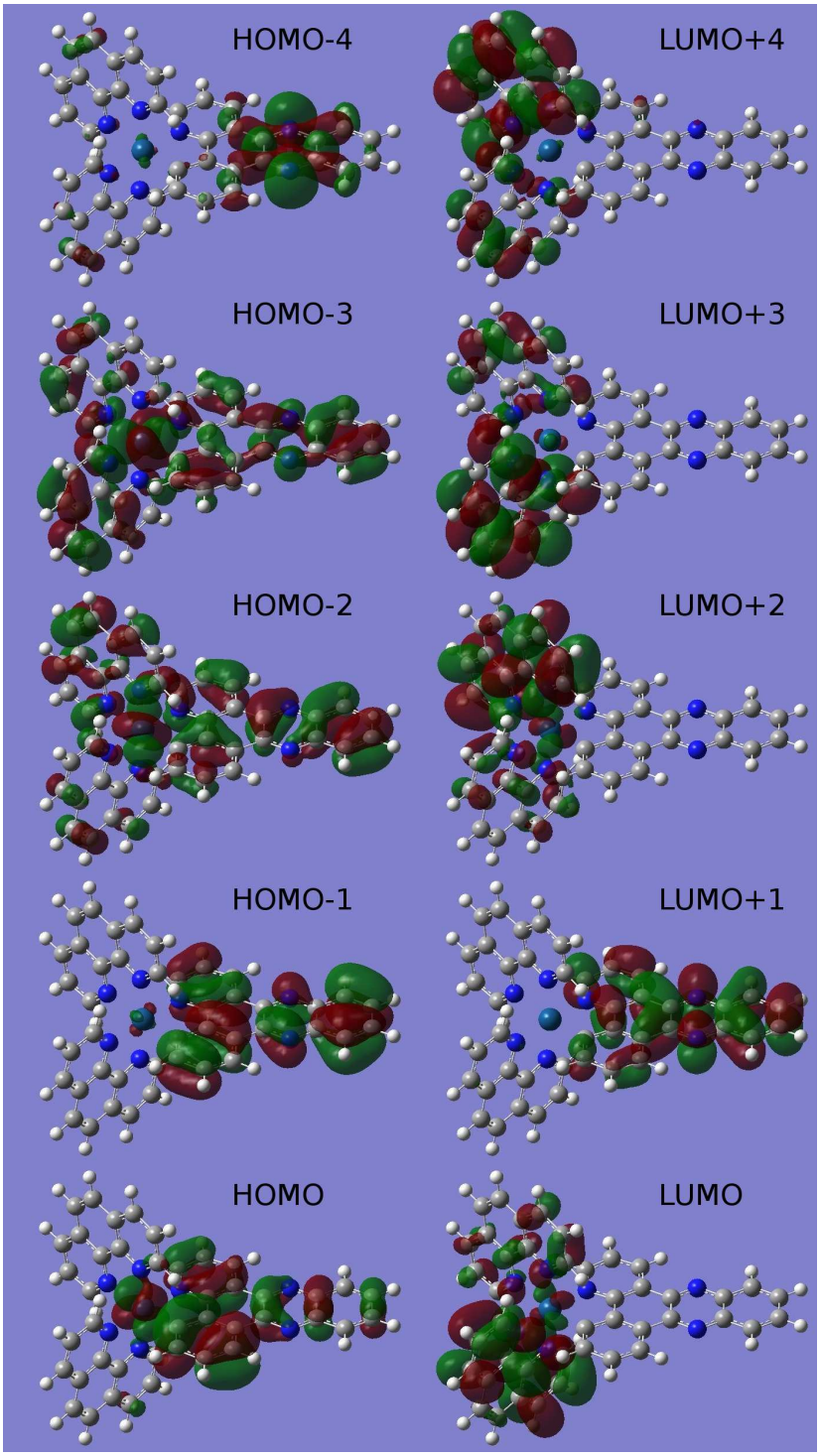
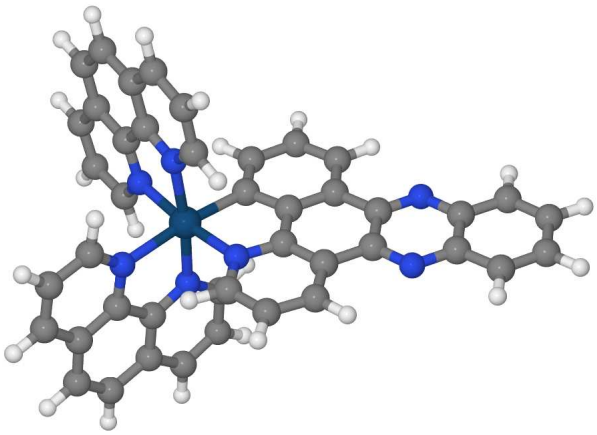


FIG. S8. Frontier orbitals for **1**

S10. $[IR(PHEN)_2(BPPZ)]^{2+}$ (T_1) [2]

S10.1. General Information



SMILES	:	c1ccc2c(c1)nc-3c(n2)-c4ccc[n+]5c4-c6c3cccc6[Ir]578([n+]9cccc1c9c2[n+]7cccc2cc1)[n+]1cccc2c1c1[n+]8cccc1cc2
Formula	:	$C_{43}H_{26}IrN_7^{2+,3}$
Charge	:	2
Multiplicity	:	3
Energy	:	-2142.29978975 a.u.
Number of imaginary frequencies	:	0

S10.2. Cartesian Co-ordinates (XYZ format)

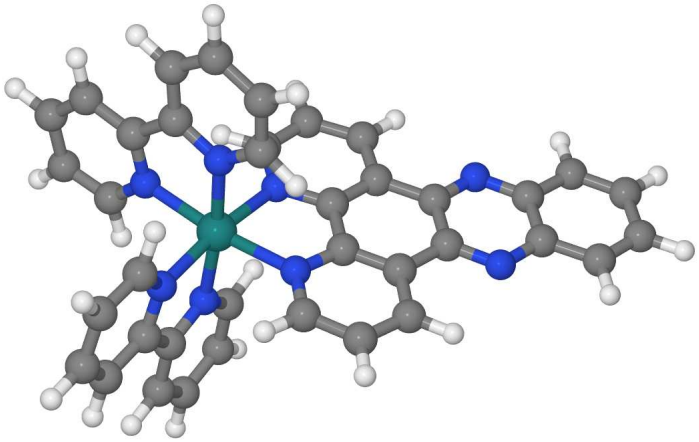
77

N	4.26813126	-0.95952785	1.03164685
N	4.26294041	0.99478763	-0.99434376
N	-0.53962457	0.87833565	-0.99169207
C	-0.64508098	-1.94120252	1.93599939
H	-1.59221363	-2.31485152	2.30675697
C	0.54835588	-2.44089246	2.48448730
H	0.49798629	-3.19173193	3.26522946
C	1.78829515	-1.99388695	2.04942918
H	2.70223689	-2.38244033	2.47799420
C	1.86291099	-1.02213442	1.03972447
C	3.13246489	-0.50006038	0.52877975
C	5.42619133	-0.46471107	0.54523498
C	6.66574383	-0.93137807	1.05712056
H	6.64683199	-1.68327236	1.83664107
C	7.84264040	-0.42925152	0.56229877
C	7.84059763	0.55716330	-0.46121562
C	6.66080666	1.02969003	-0.97742611
H	6.63675880	1.78094864	-1.75745797
C	5.42509842	0.53103924	-0.48756948
C	3.13583946	0.50195152	-0.50949740
C	1.86930835	0.99670112	-1.05188107
C	1.78529620	1.96540701	-2.05884981
H	2.69494128	2.38248587	-2.47004771
C	0.53861809	2.37149763	-2.50933266

H	0.43660015	3.11773396	-3.28516603
C	-0.60715723	1.80876660	-1.95333707
H	-1.59547353	2.09759140	-2.28120732
C	0.67866760	0.46913850	-0.53464621
C	0.66011113	-0.53167701	0.49840564
C	-3.17861462	-2.58524036	-0.94314927
C	-1.55089605	-1.85744810	-2.45856929
C	-3.42559576	-3.78029394	-1.68786025
C	-3.91707277	-2.31132936	0.27894330
C	-1.72759795	-2.99332261	-3.23826480
H	-0.84281749	-1.08401263	-2.70927191
C	-2.65137291	-3.96099663	-2.87731314
C	-4.89735556	-3.23444843	0.75939149
H	-1.12920976	-3.10707045	-4.13258600
H	-2.79547763	-4.84865141	-3.47945356
C	-4.27648449	-0.84431279	2.06065702
C	-5.56744576	-2.87756014	1.97170210
C	-5.24408960	-1.68818247	2.59918737
H	-3.99680805	0.08699162	2.52729583
H	-6.31746912	-3.54105496	2.38270640
H	-5.73512506	-1.39459693	3.51752377
N	-3.62424874	-1.16881096	0.90349883
N	-2.28611946	-1.66700673	-1.31444824
C	-3.93075347	2.31477332	-0.28666052
C	-4.39551497	0.92247081	-2.08423495
C	-4.89427233	3.26071215	-0.69275296
C	-3.15577435	2.54206204	0.89397389
C	-5.37535477	1.80837846	-2.55656886
H	-4.17233801	0.00056211	-2.60538197
C	-5.62503052	2.97512960	-1.86587930
C	-3.35138464	3.71759248	1.64751816
H	-5.91931534	1.56162822	-3.45812392
H	-6.37509108	3.67548656	-2.21272445
C	-1.49902570	1.78502369	2.34647393
C	-2.55633974	3.89493680	2.79897475
C	-1.63392377	2.93011785	3.14128590
H	-0.78955138	1.00793302	2.59266877
H	-2.67749166	4.78646278	3.40220237
H	-1.00748599	3.03455544	4.01653337
N	-3.69340277	1.17000639	-0.98330814
N	-2.24051118	1.59124005	1.25521231
H	8.78514194	0.93568391	-0.83326477
H	8.78906918	-0.78470373	0.95205659
Ir	-2.15040517	-0.05361265	-0.03407547
C	-0.60913193	-0.97661048	0.93385112
C	-5.07821846	4.44531631	0.09299174
C	-4.33750963	4.66409826	1.21315062
H	-5.82140732	5.16569090	-0.22605419
H	-4.48037195	5.56204319	1.80152690
C	-5.12632751	-4.39222050	0.02822808
C	-4.38076162	-4.66786671	-1.21096933
H	-5.86251879	-5.10957289	0.36537966
H	-4.58617640	-5.58265686	-1.75086677

S11. $[RU(BIPY)_2(DPPZ)]^{2+}$ (S_0)

S11.1. General Information



SMILES	:	c1ccc2c(c1)nc-3c(n2)-c4ccc[n+]5c4-c6c3ccc[n+]6[Ru]578([n+]9 ccccc9-c1[n+]7cccc1)[n+]1ccccc1-c1[n+]8cccc1
Formula	:	$C_{38}H_{26}N_8Ru^{2+}$
Charge	:	2
Multiplicity	:	1
Energy	:	-1997.11055479 a.u.
Number of imaginary frequencies	:	0

S11.2. Cartesian Co-ordinates (XYZ format)

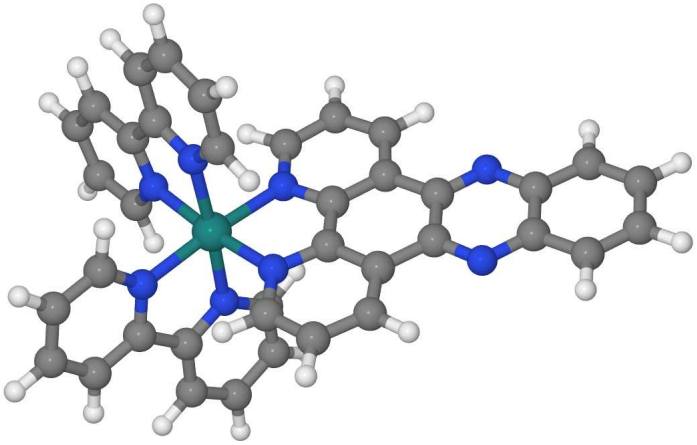
73

N	0.31218511	-0.87970018	0.99888390
N	5.12858343	-0.93535203	1.05239844
N	5.12862110	0.93497568	-1.05257308
N	0.31222019	0.87972188	-0.99887687
C	0.26408970	-1.77254391	1.99450958
H	-0.72014654	-2.06580472	2.33245397
C	1.41634917	-2.29873657	2.57956195
H	1.31999326	-3.01662397	3.38293076
C	2.65867758	-1.89390969	2.12537885
H	3.57284498	-2.27845550	2.55659080
C	2.73098207	-0.96236849	1.07984746
C	3.99954987	-0.47748193	0.53654683
C	6.28777647	-0.47693372	0.53734660
C	7.52550077	-0.93835670	1.05829871
H	7.50431824	-1.65674078	1.86853254
C	8.70267391	-0.47185308	0.53214663
C	8.70269299	0.47119999	-0.53243941
C	7.52553797	0.93779451	-1.05855274
H	7.50438452	1.65617919	-1.86878669
C	6.28779554	0.47647119	-0.53755629
C	3.99956918	0.47718924	-0.53668731
C	2.73102093	0.96218717	-1.07993436
C	2.65875411	1.89373636	-2.12546110
H	3.57293701	2.27820468	-2.55670929

C	1.41644204	2.29866719	-2.57959652
H	1.32011521	3.01656270	-3.38296127
C	0.26416111	1.77257025	-1.99450004
H	-0.72006363	2.06591439	-2.33240581
C	1.53034735	0.48087662	-0.54021770
C	1.53032792	-0.48095751	0.54017711
C	-2.33797002	-2.63440466	-0.79542214
C	-0.67670494	-1.94910157	-2.28352070
C	-2.50315499	-3.82513094	-1.50239575
C	-3.10938215	-2.28095460	0.40979615
C	-0.79713279	-3.11393976	-3.02585292
H	0.03057373	-1.18018591	-2.55985188
C	-1.72769189	-4.06906319	-2.62829399
H	-3.22819781	-4.55782986	-1.17874324
C	-4.10302019	-3.08926988	0.96095175
H	-0.17027402	-3.26018429	-3.89518046
H	-1.84894705	-4.99015045	-3.18382859
C	-3.44072270	-0.68702960	2.08166766
C	-4.77344036	-2.67247415	2.10341978
H	-4.35376215	-4.03531694	0.50365126
C	-4.43585396	-1.44922590	2.67436337
H	-3.14647985	0.26778331	2.49356914
H	-5.54600620	-3.29343462	2.53838468
H	-4.93040609	-1.08262622	3.56379676
N	-2.78643513	-1.08642054	0.97691804
N	-1.42691326	-1.70545077	-1.19464672
C	-3.10919929	2.28127313	-0.40964931
C	-3.44075084	0.68737549	-2.08150506
C	-4.10278940	3.08967519	-0.96076351
C	-2.33770537	2.63465667	0.79553622
C	-4.43584061	1.44965863	-2.67415905
H	-3.14660954	-0.26746371	-2.49341774
C	-4.77329445	2.67293739	-2.10320282
H	-4.35342932	4.03574467	-0.50345331
C	-2.50275517	3.82539868	1.50251472
H	-4.93046236	1.08310151	-3.56357121
H	-5.54582453	3.29396510	-2.53813553
C	-0.67643970	1.94920814	2.28356743
C	-1.72722363	4.06926394	2.62838054
H	-3.22774601	4.55816174	1.17889118
C	-0.79673332	3.11405826	3.02590251
H	0.03078174	1.18022978	2.55987072
H	-1.84837377	4.99036264	3.18391871
H	-0.16982573	3.26024818	3.89520431
N	-2.78638124	1.08671010	-0.97678357
N	-1.42671442	1.70562243	1.19472444
H	9.64864349	0.82132429	-0.92779189
H	9.64861107	-0.82205105	0.92746741
Ru	-1.30272555	0.00008019	0.00003645

S12. $[RU(BIPY)_2(DPPZ)]^{2+}$ (T_1)

S12.1. General Information



SMILES	:	c1ccc2c(c1)nc3=c4ccc[n+]5c4=c6c(=c3n2)ccc[n+]6[Ru]578([n+]9ccccc9-c1[n+]7cccc1)[n+]1ccccc1-c1[n+]8cccc1
Formula	:	$C_{38}H_{26}N_8Ru^{2+,3}$
Charge	:	2
Multiplicity	:	3
Energy	:	-1997.03462782 a.u.
Number of imaginary frequencies	:	0

S12.2. Cartesian Co-ordinates (XYZ format)

73

N	0.26641476	-0.91059524	0.98203224
N	5.11710405	-0.98398298	1.01135361
N	5.11715889	0.98362398	-1.01147664
N	0.26645935	0.91069049	-0.98196334
C	0.22217210	-1.86241436	1.92341483
H	-0.76108217	-2.17348862	2.25125432
C	1.37006021	-2.41552305	2.47503018
H	1.27955794	-3.17084384	3.24287653
C	2.62609410	-1.97634292	2.02838612
H	3.53678823	-2.38834786	2.44324493
C	2.71555281	-1.00702846	1.04143000
C	3.98547649	-0.50423455	0.51933873
C	6.28391504	-0.49966842	0.51257944
C	7.51824474	-0.98283887	1.00802875
H	7.49693489	-1.73895860	1.78399050
C	8.70495605	-0.49403915	0.50623024
C	8.70498371	0.49314880	-0.50667119
C	7.51830053	0.98212236	-1.00836658
H	7.49703407	1.73824608	-1.78432548
C	6.28394270	0.49912590	-0.51281673
C	3.98550344	0.50405675	-0.51934820
C	2.71560502	1.00693667	-1.04142141
C	2.62619472	1.97624373	-2.02838945
H	3.53691006	2.38817477	-2.44327497

C	1.37018311	2.41552401	-2.47499776
H	1.27971959	3.17084336	-3.24285007
C	0.22226565	1.86251044	-1.92334771
H	-0.76097208	2.17365289	-2.25117159
C	1.50032163	0.47742784	-0.50729400
C	1.50029767	-0.47742215	0.50733548
C	-2.30045962	-2.67090845	-0.76718074
C	-0.56172961	-1.99091852	-2.18287134
C	-2.39924693	-3.88418937	-1.44302857
C	-3.13162923	-2.29744554	0.38915193
C	-0.62043726	-3.17980742	-2.89291573
H	0.14583702	-1.21379876	-2.43370008
C	-1.55403340	-4.13984108	-2.51605415
H	-3.12290955	-4.62501907	-1.13637662
C	-4.14439201	-3.09566545	0.91462302
H	0.05766939	-3.34090161	-3.71957159
H	-1.62326956	-5.08026457	-3.04737616
C	-3.55994987	-0.64653611	1.99195802
C	-4.87000608	-2.64541698	2.01075339
H	-4.36765289	-4.05670738	0.47534764
C	-4.57399750	-1.40190363	2.56004333
H	-3.29399872	0.32523069	2.38343883
H	-5.65802765	-3.25925279	2.42738771
H	-5.11514330	-1.01428747	3.41210532
N	-2.85289526	-1.08471859	0.93744582
N	-1.38571382	-1.74023461	-1.15136290
C	-3.13150001	2.29775429	-0.38901269
C	-3.55997133	0.64684767	-1.99178445
C	-4.14423466	3.09602571	-0.91446048
C	-2.30026484	2.67118526	0.76728535
C	-4.57399321	1.40226781	-2.55984592
H	-3.29408813	-0.32494092	-2.38325930
C	-4.86991119	2.64580512	-2.01056099
H	-4.36742544	4.05708647	-0.47519124
C	-2.39894414	3.88448620	1.44311440
H	-5.11519051	1.01467288	-3.41188478
H	-5.65791130	3.25968170	-2.42717624
C	-0.56152630	1.99110651	2.18292451
C	-1.55367362	4.14010096	2.51610422
H	-3.12256455	4.62536144	1.13647413
C	-0.62012839	3.18001175	2.89294958
H	0.14600120	1.21394694	2.43373966
H	-1.62282348	5.08054066	3.04740882
H	0.05802232	3.34107733	3.71957517
N	-2.85285830	1.08500314	-0.93730068
N	-1.38556802	1.74045694	1.15145278
H	9.64830208	0.86547232	-0.88868588
H	9.64825249	-0.86650121	0.88816267
Ru	-1.31857967	0.00010169	0.00005253