

## SUPPORTING INFORMATION

# LIGHT-HARVESTING AND ELECTRONIC CONTACTING CAPABILITIES OF RU(II) IPA ROD AND STAR COMPLEXES - FIRST PRINCIPLES PREDICTIONS

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### Calculated TD-DFT excitations

All calculations performed using Gaussian09 (Revision A.02).  
Singlet excitations from TD-DFT calculations with pbe1pbe/sdd  
and scrf=(iefpcm,solvent=acetonitrile).

State	E/eV	$\lambda$ /nm	f
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<b>L1</b>			
1	3.8938	318.41	0.0042
2	4.0272	307.87	0.0000
3	4.2350	292.76	0.3260
4	4.2492	291.78	0.0265
5	4.4890	276.19	0.0000
6	4.5713	271.22	0.0008
7	4.6163	268.58	0.0000
8	4.6658	265.73	0.0010
9	4.9939	248.27	0.0000
10	5.3261	232.79	0.0000
<b>L2</b>			
1	4.0173	308.63	0.0279
2	4.0414	306.78	0.0030
3	4.1360	299.77	1.0644
4	4.2163	294.06	0.1593
5	4.3899	282.43	0.0000
6	4.4934	275.93	0.0002
7	4.6088	269.02	0.0008
8	4.6856	264.60	0.0002
9	4.6977	263.92	0.3051
10	4.7213	262.61	0.0000

**L3**

1	3.4781	356.47	2.1783
2	3.6339	341.18	0.0211
3	4.0382	307.03	0.0028
4	4.0828	303.67	0.0236
5	4.2075	294.68	0.0344
6	4.3888	282.50	0.0001
7	4.4151	280.82	0.2194
8	4.5367	273.29	0.0086
9	4.5734	271.10	0.0008
10	4.5952	269.81	0.0553

**L4**

1	3.3492	370.19	1.5602
2	3.5840	345.94	0.0166
3	3.9131	316.85	0.4983
4	4.0006	309.92	0.0096
5	4.0334	307.39	0.0028
6	4.1534	298.51	0.0402
7	4.2396	292.44	0.0080
8	4.3315	286.24	0.1919
9	4.3842	282.80	0.0001
10	4.4600	277.99	0.0076

**L5**

1	4.0257	307.98	0.0000
2	4.0260	307.96	0.0558
3	4.0295	307.69	0.0037
4	4.0723	304.46	2.3786
5	4.1436	299.22	0.0000
6	4.2128	294.30	0.0000
7	4.2168	294.02	0.0000
8	4.2650	290.70	0.1258
9	4.3670	283.91	0.1321
10	4.4806	276.71	0.0000

**L6**

1	3.4196	362.57	4.5184
2	3.5183	352.39	0.0000
3	3.6378	340.82	0.0002
4	3.6378	340.82	0.0419
5	3.7427	331.27	0.0000
6	3.7502	330.60	0.0050
7	4.0856	303.47	0.0000
8	4.0856	303.47	0.0001
9	4.1140	301.37	0.0000
10	4.1214	300.83	0.0257

**L7**

1	3.2573	380.64	2.3407
2	3.4273	361.76	1.1450

3	3.5089	353.35	0.0247
4	3.5228	351.95	0.0117
5	3.6352	341.07	0.0192
6	3.7592	329.81	0.0134
7	3.8755	319.92	0.6197
8	3.8770	319.80	0.0009
9	3.9209	316.21	0.0083
10	4.0743	304.31	0.0002

**L8**

1	3.8261	324.05	2.9356
2	3.9391	314.75	0.0000
3	3.9867	311.00	0.0036
4	4.0283	307.79	0.0000
5	4.0936	302.87	0.0016
6	4.1377	299.65	0.0000
7	4.1938	295.64	0.1441
8	4.2687	290.45	0.0000
9	4.4994	275.56	0.0000
10	4.5217	274.20	0.0000

**L9**

1	3.2213	384.89	3.3217
2	3.3185	373.62	0.0000
3	3.5068	353.55	0.0000
4	3.5212	352.11	0.0284
5	3.7628	329.50	0.0000
6	3.7634	329.45	0.0557
7	3.8071	325.67	0.0023
8	3.8614	321.09	0.0000
9	4.2224	293.64	0.0000
10	4.2423	292.26	0.0002

**RuN3-L1**

1	1.6419	755.13	0.0264
2	1.8999	652.59	0.0005
3	2.1213	584.47	0.0650
4	2.2173	559.17	0.0243
5	2.4427	507.57	0.1736
6	2.5200	492.00	0.0100
7	2.5909	478.54	0.0344
8	2.6542	467.13	0.0812
9	2.6943	460.18	0.0371
10	2.7818	445.70	0.0277
11	2.8066	441.77	0.0368
12	3.0581	405.43	0.0050
13	3.1094	398.74	0.0009
14	3.2439	382.21	0.0076
15	3.2752	378.56	0.0368
16	3.3007	375.63	0.0082
17	3.3099	374.59	0.0043

18	3.3972	364.96	0.0416
19	3.4440	360.00	0.0603
20	3.5018	354.05	0.0589
21	3.6041	344.01	0.0043
22	3.6405	340.57	0.0076
23	3.7009	335.01	0.0124
24	3.7318	332.24	0.0095
25	3.7904	327.10	0.0574
26	3.8192	324.63	0.0052
27	3.8437	322.56	0.0301
28	3.8799	319.55	0.0088
29	3.9186	316.40	0.0266
30	3.9764	311.80	0.0327
31	4.0173	308.62	0.0064
32	4.1033	302.16	0.0727
33	4.1076	301.84	0.0311
34	4.1514	298.66	0.1607
35	4.2644	290.74	0.0022
36	4.2671	290.56	0.0025
37	4.3233	286.78	0.0866
38	4.3356	285.97	0.0032
39	4.3489	285.09	0.0007
40	4.3604	284.34	0.0106

**RuN3-L2**

1	1.8998	652.60	0.0936
2	2.1000	590.41	0.0198
3	2.1582	574.48	0.0040
4	2.3103	536.66	0.1920
5	2.3947	517.74	0.0045
6	2.5606	484.20	0.0648
7	2.6562	466.78	0.1750
8	2.7423	452.12	0.0010
9	2.9298	423.19	0.0130
10	2.9667	417.93	0.0057
11	3.0674	404.20	0.0001
12	3.1007	399.86	0.0126
13	3.1166	397.82	0.0000
14	3.1265	396.56	0.0571
15	3.2331	383.49	0.0023
16	3.3454	370.61	0.0300
17	3.3810	366.71	0.0203
18	3.3832	366.47	0.0265
19	3.4284	361.64	0.0295
20	3.4453	359.86	0.0152
21	3.5166	352.57	0.0775
22	3.5371	350.53	0.0454
23	3.5557	348.69	0.0009
24	3.5906	345.30	0.0036
25	3.6253	342.00	0.0422
26	3.6581	338.93	0.0337

27	3.6846	336.50	0.0580
28	3.7129	333.93	0.1622
29	3.7467	330.91	0.0012
30	3.7540	330.27	0.0113
31	3.7646	329.35	0.0025
32	3.7948	326.72	0.0660
33	3.8280	323.88	0.0055
34	3.9810	311.44	0.0480
35	4.0921	302.98	0.0787
36	4.0946	302.80	0.0167
37	4.1042	302.09	0.5633
38	4.1899	295.91	0.0045
39	4.2117	294.38	0.1134
40	4.2280	293.24	0.0041

### **RuN3-L3**

1	1.9018	651.92	0.1421
2	2.0912	592.90	0.0219
3	2.1678	571.93	0.0035
4	2.3049	537.91	0.2797
5	2.3858	519.67	0.0057
6	2.5454	487.10	0.1066
7	2.6094	475.15	0.2187
8	2.8892	429.12	0.0003
9	2.8983	427.78	0.0126
10	2.9300	423.15	0.0102
11	3.0587	405.34	0.0100
12	3.1194	397.46	0.1432
13	3.2164	385.48	0.1357
14	3.2166	385.45	0.0070
15	3.2244	384.51	0.0006
16	3.2529	381.15	0.0001
17	3.3338	371.90	0.2540
18	3.3538	369.68	1.0498
19	3.3779	367.05	0.0113
20	3.3965	365.03	0.0216
21	3.4086	363.74	0.1267
22	3.4898	355.28	0.0263
23	3.5155	352.67	0.0022
24	3.5340	350.83	0.0185
25	3.5438	349.86	0.0220
26	3.5691	347.38	0.0047
27	3.6079	343.65	0.0081
28	3.6363	340.96	0.0423
29	3.6623	338.54	0.0386
30	3.7004	335.06	0.0239
31	3.7019	334.92	0.0205
32	3.7572	329.99	0.0540
33	3.7974	326.50	0.0491
34	3.8172	324.80	0.0104
35	3.8481	322.20	0.0053

36	3.8936	318.43	0.0940
37	3.9026	317.70	0.0006
38	3.9092	317.16	0.1545
39	4.0873	303.34	0.0016
40	4.1151	301.29	0.0173

#### **RuN3-L4**

1	1.8639	665.17	0.0079
2	2.0993	590.61	0.0291
3	2.1627	573.28	0.0149
4	2.3125	536.15	0.3916
5	2.3720	522.70	0.0008
6	2.5371	488.68	0.1008
7	2.6583	466.40	0.0731
8	2.8290	438.25	0.2458
9	2.9028	427.12	0.0118
10	2.9113	425.88	0.0000
11	3.0549	405.85	0.0246
12	3.1085	398.86	0.0267
13	3.1553	392.93	0.0009
14	3.1704	391.07	0.0310
15	3.1843	389.36	1.0168
16	3.2344	383.34	0.0000
17	3.2912	376.71	0.0272
18	3.3129	374.25	0.0075
19	3.3671	368.23	0.0097
20	3.3739	367.48	0.0169
21	3.4097	363.63	0.0603
22	3.4323	361.23	0.0122
23	3.4843	355.83	0.0033
24	3.5462	349.63	0.0024
25	3.5562	348.64	0.0078
26	3.5779	346.53	0.0151
27	3.5875	345.60	0.0161
28	3.6302	341.53	0.0277
29	3.6438	340.26	0.0146
30	3.6649	338.30	0.0080
31	3.6886	336.13	0.0351
32	3.6920	335.82	0.0531
33	3.7189	333.39	0.0177
34	3.7379	331.70	0.2939
35	3.7775	328.22	0.2785
36	3.8132	325.14	0.0554
37	3.8459	322.38	0.0024
38	3.8845	319.17	0.0000
39	3.9657	312.64	0.0013
40	4.0020	309.81	0.0134

#### **RuN3-L5**

1	1.7732	699.21	0.0520
2	2.0528	603.98	0.0015

3	2.1269	582.94	0.0514
4	2.2164	559.40	0.1258
5	2.4107	514.31	0.0201
6	2.4580	504.40	0.2543
7	2.6085	475.32	0.1403
8	2.7228	455.35	0.0899
9	2.7377	452.87	0.0142
10	2.7524	450.46	0.1035
11	2.7851	445.16	0.0005
12	2.8001	442.79	0.0002
13	2.9927	414.29	0.0371
14	3.0231	410.12	0.0234
15	3.0650	404.52	0.0014
16	3.0873	401.59	0.0004
17	3.0947	400.63	0.0023
18	3.1409	394.74	0.0000
19	3.1582	392.58	0.0001
20	3.1909	388.55	0.0080
21	3.3260	372.77	0.0262
22	3.3457	370.58	0.0781
23	3.3634	368.62	0.0704
24	3.4128	363.30	0.0151
25	3.4319	361.27	0.0015
26	3.4540	358.95	0.0717
27	3.4892	355.34	0.0157
28	3.4963	354.61	0.0908
29	3.5390	350.33	0.0079
30	3.5729	347.01	0.1021
31	3.6000	344.40	0.0172
32	3.6563	339.10	0.0257
33	3.6839	336.56	0.0148
34	3.7113	334.07	0.0414
35	3.7357	331.89	0.0161
36	3.7582	329.90	0.0000
37	3.7603	329.72	0.0033
38	3.7782	328.16	0.0003
39	3.7867	327.42	0.0261
40	3.7920	326.96	0.0838
41	3.8450	322.46	0.0322
42	3.8774	319.76	0.4476
43	3.9253	315.86	0.2900
44	3.9705	312.26	0.1135
45	4.0217	308.29	0.0237
46	4.0304	307.62	0.0211
47	4.0798	303.89	0.0853
48	4.0910	303.06	0.2166
49	4.1066	301.91	0.0266
50	4.1590	298.11	0.1215
51	4.1754	296.94	0.0357
52	4.2167	294.03	0.0008
53	4.2307	293.06	0.0107

54	4.2379	292.56	0.0078
55	4.2739	290.09	0.0291
56	4.2990	288.40	0.0006
57	4.3168	287.21	0.0012
58	4.3224	286.84	0.0027
59	4.3350	286.01	0.0517
60	4.3569	284.57	0.0015

**RuN3-L6**

1	1.7828	695.46	0.0761
2	2.0656	600.23	0.0031
3	2.1153	586.14	0.0689
4	2.2078	561.57	0.1783
5	2.3873	519.35	0.0666
6	2.4110	514.24	0.3733
7	2.5812	480.34	0.2321
8	2.6723	463.97	0.2145
9	2.6995	459.28	0.0564
10	2.7112	457.30	0.0707
11	2.9237	424.06	0.0003
12	2.9332	422.70	0.0000
13	2.9768	416.51	0.0516
14	3.0030	412.87	0.0831
15	3.0610	405.04	0.0027
16	3.1032	399.53	0.0083
17	3.1896	388.71	0.0360
18	3.1957	387.97	0.0011
19	3.2130	385.88	0.0001
20	3.2294	383.92	0.5839
21	3.2524	381.21	0.3381
22	3.2742	378.67	0.0000
23	3.2833	377.62	0.0001
24	3.2965	376.11	1.0012
25	3.3470	370.44	0.1118
26	3.3693	367.99	0.0577
27	3.4006	364.59	0.0135
28	3.4172	362.82	0.0390
29	3.4546	358.89	0.0462
30	3.4657	357.75	0.0569
31	3.4794	356.34	0.0241
32	3.5089	353.34	0.3649
33	3.5234	351.89	0.0342
34	3.5305	351.18	0.1399
35	3.5774	346.58	0.0305
36	3.6072	343.72	0.5697
37	3.6176	342.72	0.0569
38	3.6380	340.80	0.2554
39	3.6505	339.63	0.0255
40	3.7058	334.57	0.0224
41	3.7097	334.22	0.0216
42	3.7234	332.98	0.0254



43	3.7480	330.80	0.0181
44	3.7758	328.36	0.0155
45	3.8002	326.26	0.0029
46	3.8493	322.09	0.0528
47	3.8622	321.02	0.0047
48	3.8930	318.48	0.0068
49	3.8949	318.33	0.0001
50	3.9115	316.97	0.0005
51	3.9556	313.44	0.0795
52	3.9650	312.69	0.0070
53	3.9929	310.51	0.0153
54	4.0178	308.59	0.0581
55	4.0656	304.96	0.0191
56	4.0838	303.60	0.0002
57	4.0839	303.59	0.0065
58	4.0971	302.62	0.0018
59	4.1162	301.21	0.0000
60	4.1251	300.56	0.0414

**RuN3-L7**

1	1.7777	697.46	0.0787
2	2.0589	602.18	0.0027
3	2.1130	586.77	0.0760
4	2.1930	565.36	0.1754
5	2.3807	520.80	0.2281
6	2.3950	517.68	0.2111
7	2.5725	481.96	0.2654
8	2.6549	467.00	0.1851
9	2.6802	462.60	0.0321
10	2.7006	459.09	0.0604
11	2.9176	424.95	0.0003
12	2.9273	423.54	0.0000
13	2.9635	418.36	0.0671
14	2.9894	414.74	0.0845
15	3.0508	406.40	0.0028
16	3.0899	401.26	0.0164
17	3.1098	398.69	0.6293
18	3.1763	390.34	0.0535
19	3.1830	389.52	0.0012
20	3.2040	386.97	0.0002
21	3.2381	382.89	0.1401
22	3.2632	379.94	0.8751
23	3.2702	379.13	0.0000
24	3.2771	378.34	0.0001
25	3.3408	371.12	0.0407
26	3.3606	368.94	0.0227
27	3.3884	365.91	0.0158
28	3.4017	364.48	0.1109
29	3.4128	363.30	0.3107
30	3.4305	361.42	0.0127
31	3.4464	359.75	0.0017

32	3.4712	357.18	0.0122
33	3.4960	354.64	0.1083
34	3.5079	353.45	0.0272
35	3.5264	351.59	0.0232
36	3.5771	346.61	0.0069
37	3.5900	345.36	0.2689
38	3.6170	342.79	0.0439
39	3.6445	340.19	0.0143
40	3.6480	339.87	0.0474

**RuN3-L8**

1	1.7424	711.56	0.0604
2	2.0241	612.53	0.0023
3	2.1241	583.69	0.0808
4	2.1692	571.56	0.0778
5	2.3576	525.90	0.3573
6	2.4110	514.25	0.0091
7	2.5556	485.15	0.2052
8	2.6175	473.67	0.0649
9	2.6410	469.46	0.0493
10	2.6899	460.92	0.0457
11	2.9474	420.66	0.0414
12	2.9608	418.76	0.0177
13	3.0383	408.07	0.0011
14	3.1756	390.42	0.0088
15	3.3069	374.92	0.2045
16	3.3126	374.28	0.0228
17	3.3359	371.66	0.0226
18	3.3899	365.74	0.0396
19	3.3943	365.27	0.0379
20	3.4303	361.44	0.0431
21	3.4704	357.26	0.0279
22	3.4963	354.61	0.1514
23	3.5151	352.72	0.0223
24	3.5504	349.21	0.1165
25	3.5923	345.14	0.0164
26	3.6524	339.46	0.1464
27	3.6773	337.16	0.4076
28	3.7085	334.32	0.0719
29	3.7550	330.18	0.0482
30	3.7660	329.22	0.0378
31	3.7753	328.41	0.1018
32	3.7856	327.51	0.0219
33	3.7925	326.92	0.2730
34	3.8105	325.38	0.0472
35	3.8317	323.57	0.1427
36	3.8776	319.74	0.1467
37	3.9396	314.71	0.0005
38	3.9795	311.55	0.2766
39	4.0480	306.28	0.0760
40	4.0856	303.46	0.0036

**RuN3-L9**

1	1.6069	771.58	0.0834
2	1.8694	663.23	0.0823
3	1.9015	652.04	0.0076
4	2.0219	613.20	0.3841
5	2.1428	578.62	0.1094
6	2.1748	570.10	0.1765
7	2.2099	561.04	0.0106
8	2.3127	536.11	0.0433
9	2.4268	510.90	0.0007
10	2.5749	481.52	0.0680
11	2.6225	472.78	0.0113
12	2.6501	467.85	0.0091
13	2.7241	455.14	0.0344
14	2.8686	432.21	0.0272
15	2.9407	421.62	0.0408
16	2.9864	415.16	0.1590
17	3.0992	400.05	0.7148
18	3.1604	392.31	0.3501
19	3.2072	386.58	0.0173
20	3.2245	384.51	0.2138
21	3.2450	382.07	0.0093
22	3.2473	381.81	0.6177
23	3.2614	380.16	0.0666
24	3.2961	376.15	0.0534
25	3.3057	375.07	0.0022
26	3.3533	369.74	0.1237
27	3.3598	369.03	0.1456
28	3.3940	365.31	0.0394
29	3.4074	363.87	0.1023
30	3.4498	359.39	0.0253
31	3.4885	355.41	0.1995
32	3.5400	350.24	0.0086
33	3.5923	345.14	0.0277
34	3.6222	342.29	0.1967
35	3.6630	338.48	0.0768
36	3.6696	337.87	0.1941
37	3.6839	336.56	0.0420
38	3.7525	330.41	0.0430
39	3.7683	329.02	0.0156
40	3.7919	326.97	0.0080

**RuStar-L2**

1	2.4379	508.57	0.0179
2	2.4386	508.43	0.0177
3	2.4406	508.01	0.0175
4	2.5959	477.61	0.0049
5	2.6256	472.20	0.1109
6	2.6268	471.99	0.1099
7	2.7443	451.79	0.4338

8	2.7445	451.76	0.4336
9	3.0281	409.45	0.0177
10	3.3423	370.95	0.0792
11	3.3511	369.98	0.2540
12	3.3518	369.91	0.2562
13	3.3934	365.36	0.0682
14	3.3945	365.25	0.0690
15	3.5144	352.79	0.1928
16	3.5176	352.46	0.0294
17	3.5180	352.43	0.0350
18	3.5422	350.02	0.0190
19	3.7006	335.04	0.0051
20	3.7012	334.98	0.0051
21	3.7017	334.94	0.0051
22	3.7659	329.23	0.0456
23	3.8045	325.89	0.0025
24	3.8050	325.84	0.0026
25	3.8052	325.82	0.0026
26	3.8147	325.02	0.1545
27	3.8159	324.92	0.1556
28	3.8588	321.30	0.2774
29	3.8591	321.27	0.2821
30	3.8730	320.13	0.0001
31	3.8740	320.04	0.0001
32	3.8745	320.00	0.0001
33	3.9228	316.06	0.5893
34	3.9409	314.61	0.2995
35	3.9410	314.60	0.2959
36	4.0492	306.19	0.0009
37	4.0666	304.88	0.0172
38	4.0670	304.85	0.0171
39	4.1047	302.05	0.0587
40	4.1051	302.03	0.0593

#### **RuStar-L5**

1	2.3652	524.21	0.0615
2	2.3745	522.15	0.0054
3	2.3758	521.86	0.0052
4	2.5051	494.93	0.0214
5	2.5247	491.09	0.1483
6	2.5251	491.00	0.1444
7	2.6463	468.52	0.5514
8	2.6469	468.41	0.5599
9	2.8923	428.67	0.0000
10	3.1557	392.89	0.2841
11	3.1560	392.85	0.2865
12	3.2515	381.31	0.3956
13	3.2525	381.19	0.1977
14	3.2533	381.11	0.2076
15	3.2653	379.70	0.6281
16	3.2749	378.59	0.0407

17	3.2752	378.55	0.0425
18	3.3156	373.94	0.0895
19	3.4438	360.02	0.0105
20	3.4451	359.89	0.0104
21	3.5274	351.49	0.0000
22	3.5777	346.55	0.0510
23	3.5777	346.54	0.0510
24	3.6841	336.54	0.4279
25	3.6849	336.46	0.4300
26	3.7091	334.27	0.0981
27	3.7093	334.25	0.0966
28	3.7175	333.51	0.0228
29	3.7311	332.30	0.0001
30	3.7489	330.72	0.1828
31	3.7496	330.66	0.0094
32	3.7499	330.63	0.0215
33	3.7503	330.60	0.0260
34	3.7505	330.58	0.0082
35	3.7508	330.55	0.0357
36	3.7522	330.43	0.7198
37	3.8345	323.34	0.0022
38	3.8356	323.25	0.0024
39	3.8357	323.24	0.0024
40	3.8360	323.22	0.0018

**RuStar-L6**

1	2.3225	533.85	0.1621
2	2.3412	529.58	0.0095
3	2.3422	529.34	0.0095
4	2.4417	507.78	0.4824
5	2.4420	507.72	0.4823
6	2.4480	506.47	0.0623
7	2.5558	485.12	0.9568
8	2.5558	485.10	0.9815
9	2.8055	441.94	0.0000
10	3.0106	411.83	0.2463
11	3.0109	411.78	0.2170
12	3.0260	409.73	2.4105
13	3.0282	409.43	1.8549
14	3.0287	409.36	1.8622
15	3.1217	397.17	0.0505
16	3.1220	397.13	0.1363
17	3.1227	397.04	0.0867
18	3.1255	396.68	0.0666
19	3.1258	396.65	0.0473
20	3.1602	392.33	0.0001
21	3.1794	389.96	0.1300
22	3.2504	381.45	0.1434
23	3.2512	381.35	0.1617
24	3.2532	381.11	0.0069
25	3.2957	376.20	0.0568

26	3.3146	374.05	0.2140
27	3.3153	373.98	0.2003
28	3.3184	373.63	0.0020
29	3.3245	372.94	0.1574
30	3.3248	372.91	0.1900
31	3.3456	370.58	0.0001
32	3.3638	368.58	0.0235
33	3.3640	368.56	0.0228
34	3.3874	366.02	0.0213
35	3.3881	365.94	0.0226
36	3.4726	357.04	0.0454
37	3.4749	356.80	0.2432
38	3.4749	356.80	0.2237
39	3.4859	355.67	0.0356
40	3.4861	355.65	0.0378

**RuStar-L8**

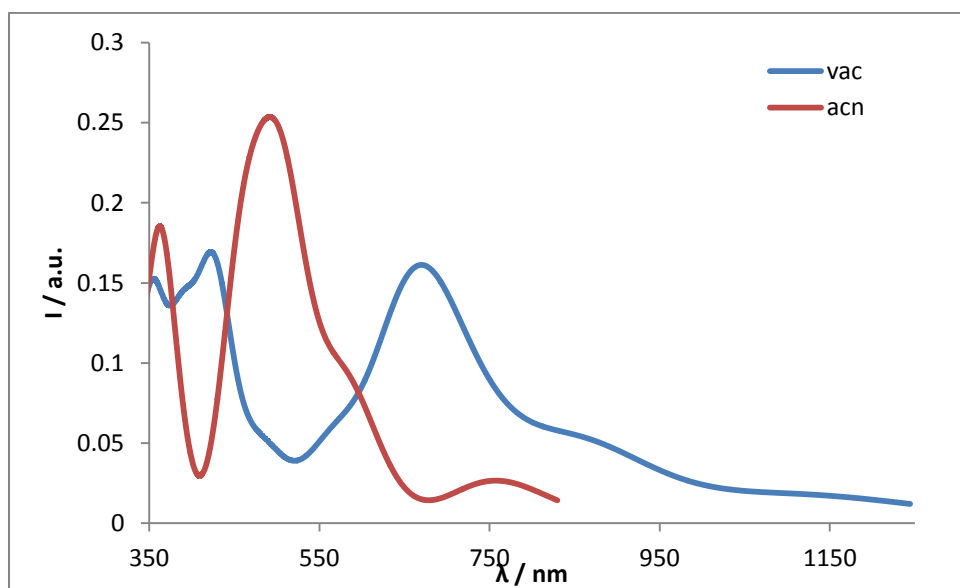
1	2.3395	529.96	0.0796
2	2.3506	527.46	0.0066
3	2.3511	527.35	0.0065
4	2.4756	500.82	0.0282
5	2.4908	497.76	0.1983
6	2.4912	497.69	0.1917
7	2.6078	475.44	0.6375
8	2.6081	475.39	0.6488
9	2.8412	436.38	0.0000
10	3.0555	405.78	0.3478
11	3.0562	405.68	0.3509
12	3.1408	394.75	0.4194
13	3.1419	394.62	0.4120
14	3.1474	393.92	0.7935
15	3.1539	393.11	0.0002
16	3.1695	391.18	0.0945
17	3.1697	391.15	0.0919
18	3.2858	377.33	0.0885
19	3.4074	363.87	0.0102
20	3.4085	363.75	0.0105
21	3.4429	360.12	0.0000
22	3.5182	352.41	0.1617
23	3.5190	352.33	0.1673
24	3.5382	350.41	0.3877
25	3.5391	350.33	0.4041
26	3.6049	343.93	0.9796
27	3.6223	342.28	0.0001
28	3.6418	340.45	0.0618
29	3.6420	340.43	0.0601
30	3.6561	339.12	0.0280
31	3.7111	334.09	0.2427
32	3.7113	334.07	0.2513
33	3.7134	333.88	0.0052
34	3.7908	327.06	0.0009

35	3.8031	326.01	0.3792
36	3.8033	325.99	0.3795
37	3.8199	324.58	0.0001
38	3.8492	322.10	0.0002
39	3.8498	322.05	0.0002
40	3.9057	317.44	0.0512

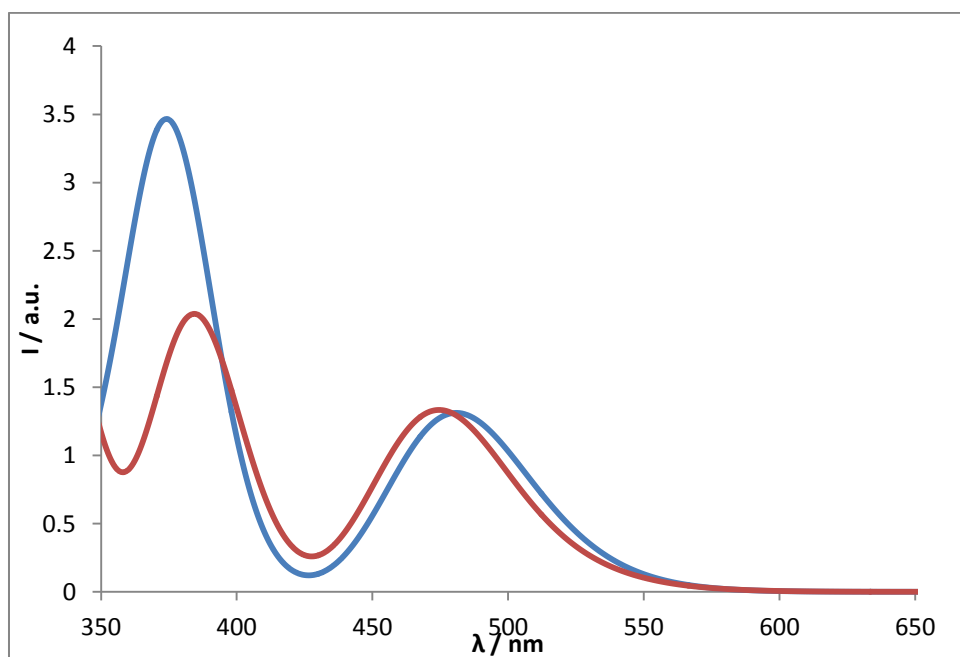
**RuStar-L9**

1	2.2763	544.69	0.1323
2	2.2892	541.62	0.0129
3	2.2897	541.48	0.0093
4	2.4047	515.59	0.1158
5	2.4090	514.67	0.3686
6	2.4104	514.38	0.4488
7	2.5085	494.25	0.8598
8	2.5089	494.17	0.9790
9	2.6805	462.55	0.0002
10	2.7580	449.55	0.4057
11	2.7604	449.16	0.4385
12	2.8099	441.25	0.7112
13	2.8112	441.03	0.4325
14	2.8113	441.02	0.4535
15	2.8565	434.04	0.0075
16	2.8639	432.92	0.1007
17	2.8661	432.58	0.1248
18	3.0538	406.00	0.0029
19	3.1110	398.53	0.1615
20	3.1620	392.11	0.1304
21	3.1633	391.94	0.1010
22	3.2225	384.74	0.0007
23	3.2240	384.57	0.0005
24	3.2458	381.98	0.4612
25	3.2476	381.78	0.5807
26	3.2751	378.57	0.3342
27	3.2884	377.03	0.0281
28	3.2894	376.93	0.0149
29	3.3055	375.09	0.5499
30	3.3265	372.71	0.0006
31	3.3804	366.77	0.0889
32	3.3849	366.28	1.0009
33	3.3873	366.03	1.1756
34	3.4664	357.67	0.5322
35	3.4705	357.25	0.6064
36	3.4789	356.38	0.0105
37	3.4908	355.17	0.0031
38	3.5350	350.74	0.1561
39	3.5375	350.48	0.1730
40	3.5525	349.01	0.0915

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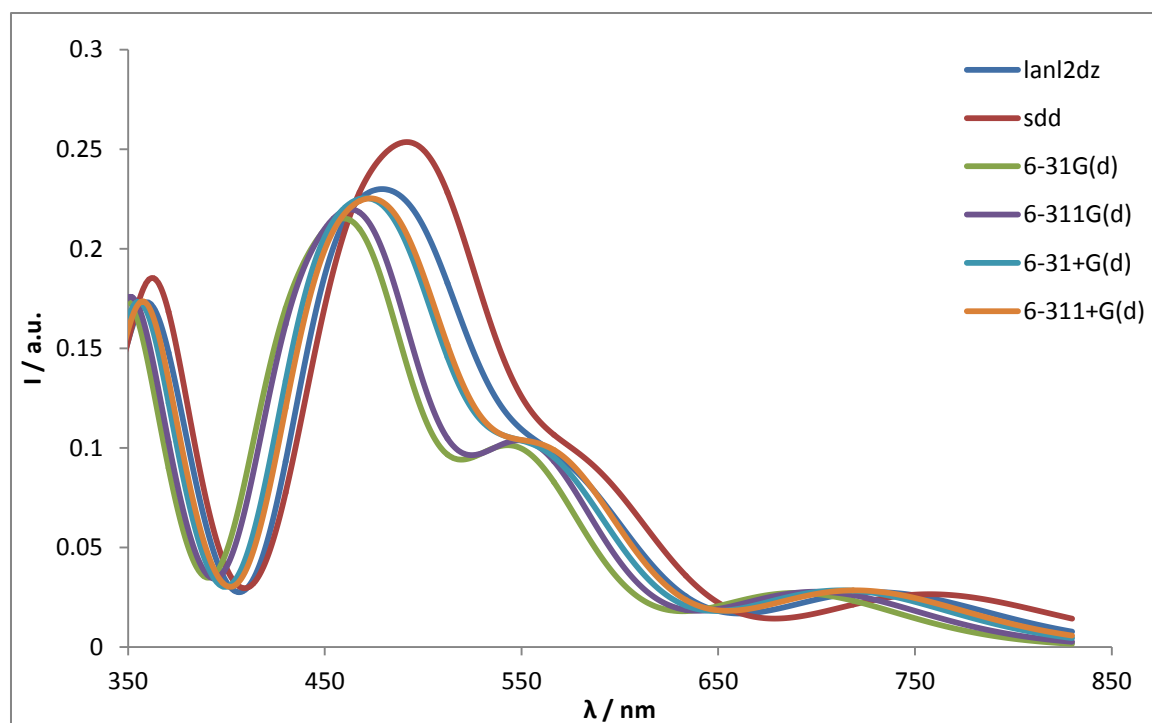


**Figure S1.** Calculated absorption spectra for RuN3-L1 with PBE0/SDD in vacuum (blue) and in acetonitrile (red).

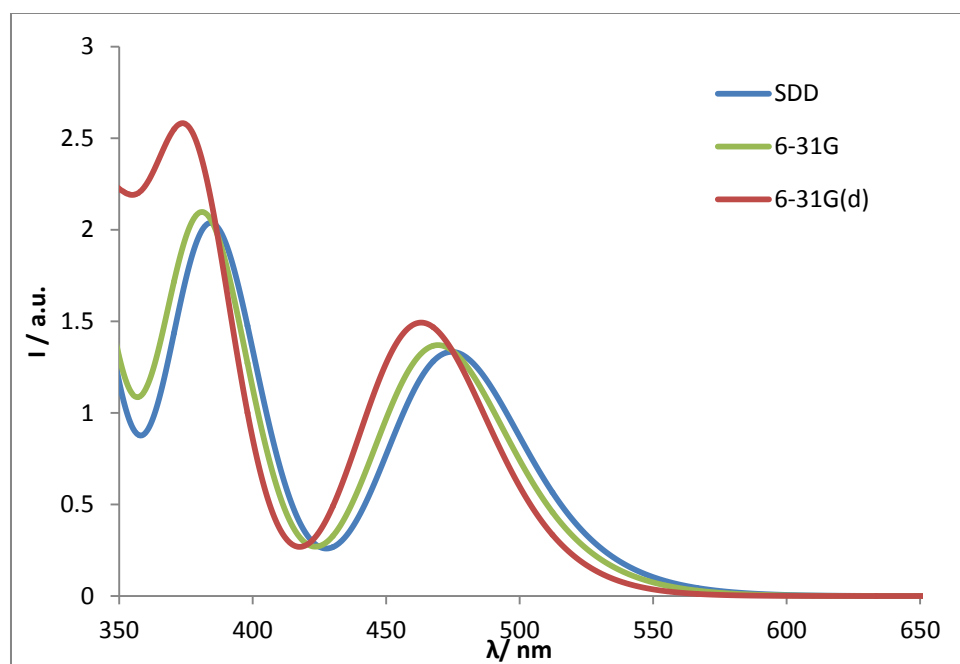


**Figure S2.** Calculated absorption spectra for RuStar-L5 with PBE0/SDD in vacuum (blue) and in acetonitrile (red).





**Figure S3.** Calculated absorption spectra for RuN3-L1 with PBE0 in acetonitrile using different basis sets.



**Figure S4.** Calculated absorption spectra for RuStar-L5 with PBE0 in acetonitrile using different basis sets.