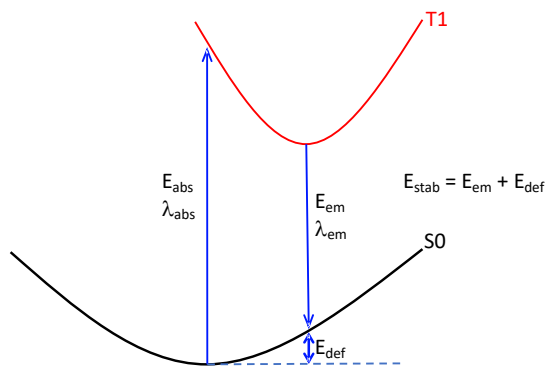Electronic Supplementary Informations

Are luminescent Ru^{2+} chelated complexes selective coordinative sensors for the detection of heavy cations ?

C. Gourlaouen, B. Schweitzer and C. Daniel

E_{abs}
λ_{abs}

E_{em}
λ_{em}

$E_{stab} = E_{em} + E_{def}$

T1

S0

E_{def}

Scheme S1: Definition of E_{abs}, E_{em}, E_{def} and E_{stab} energies.
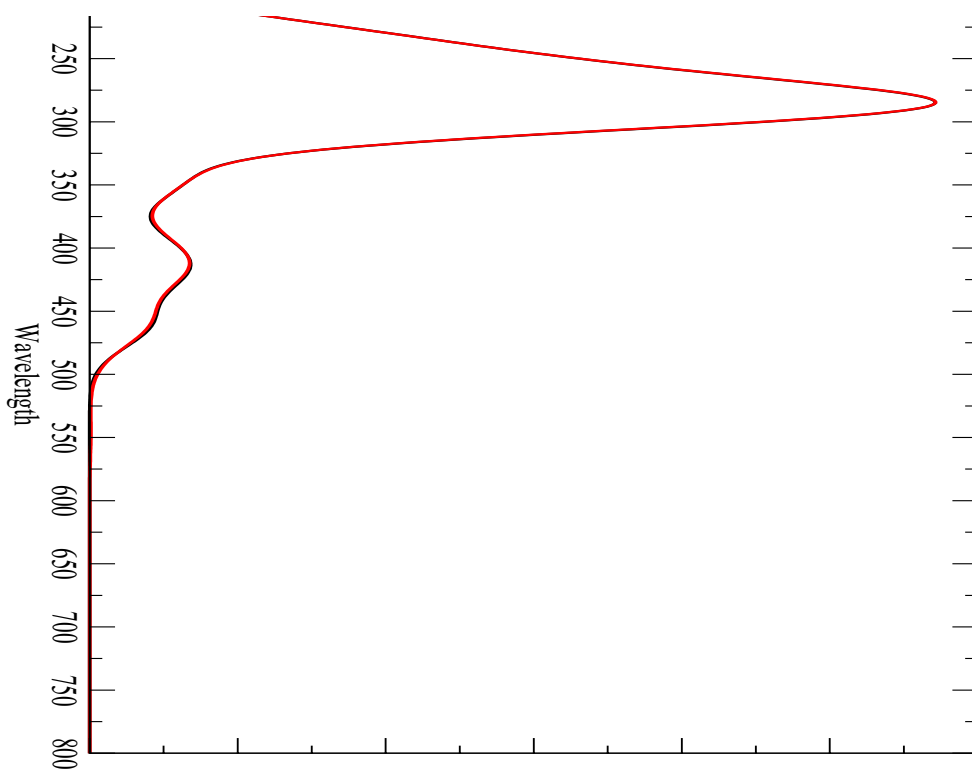
*Figure S1 : spectra of **1**, in black without SOC, in red with SOC*
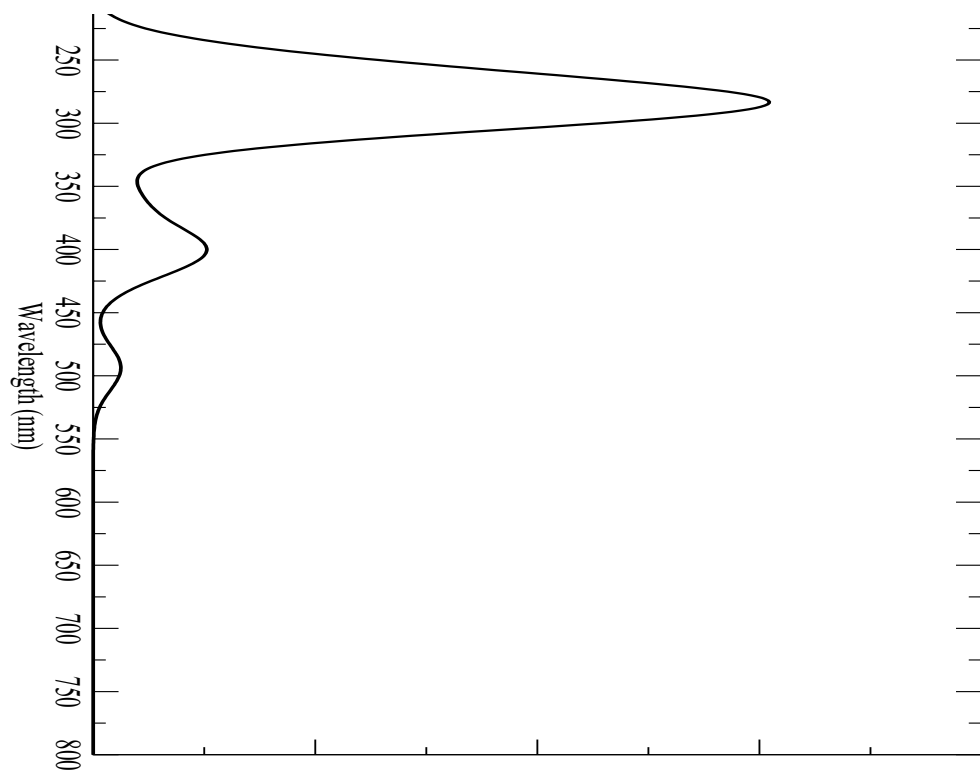
*Figure S2: spectra of **1-Ca***
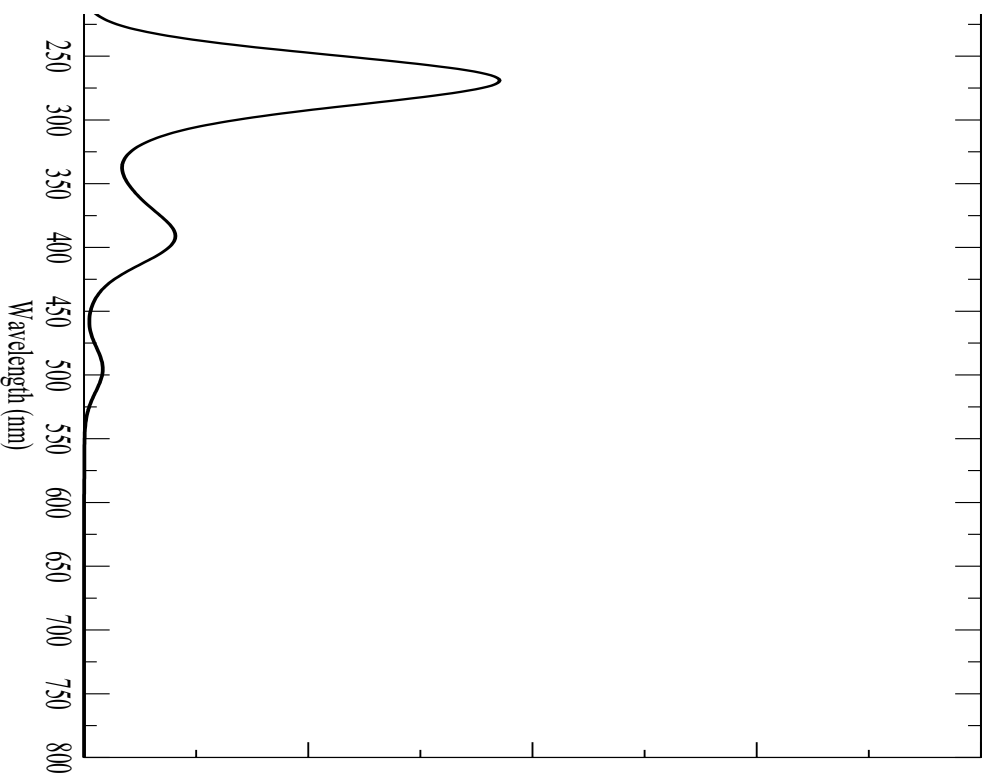
*Figure S3: spectra of **1-Mn***
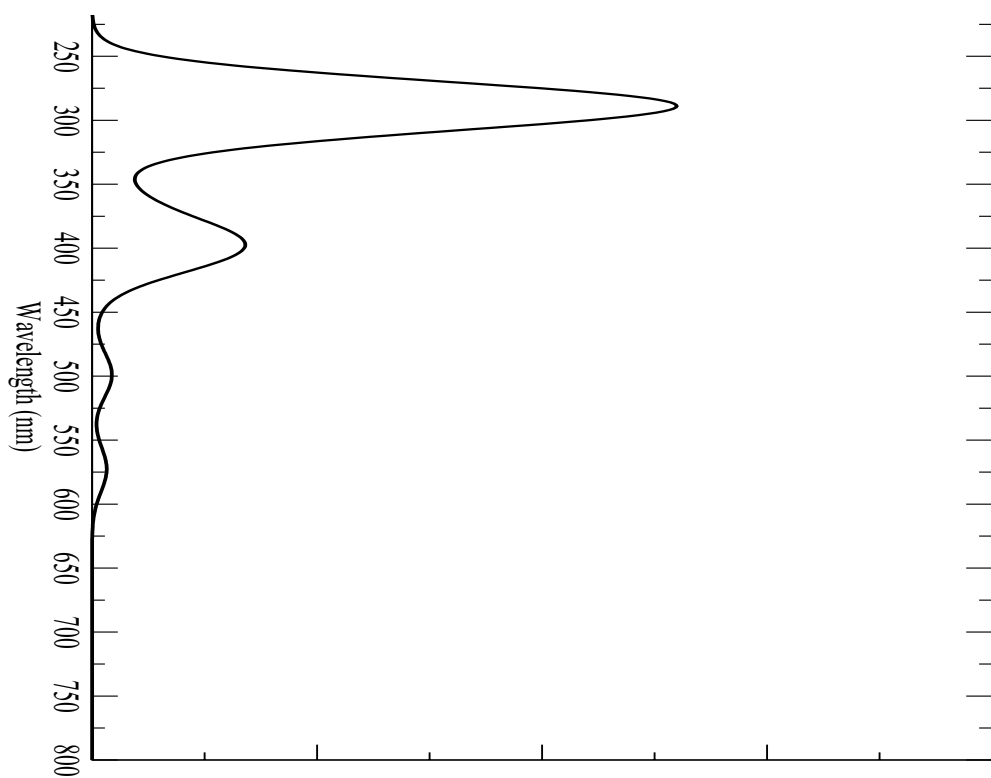
*Figure S4: spectra of **1-Fe***
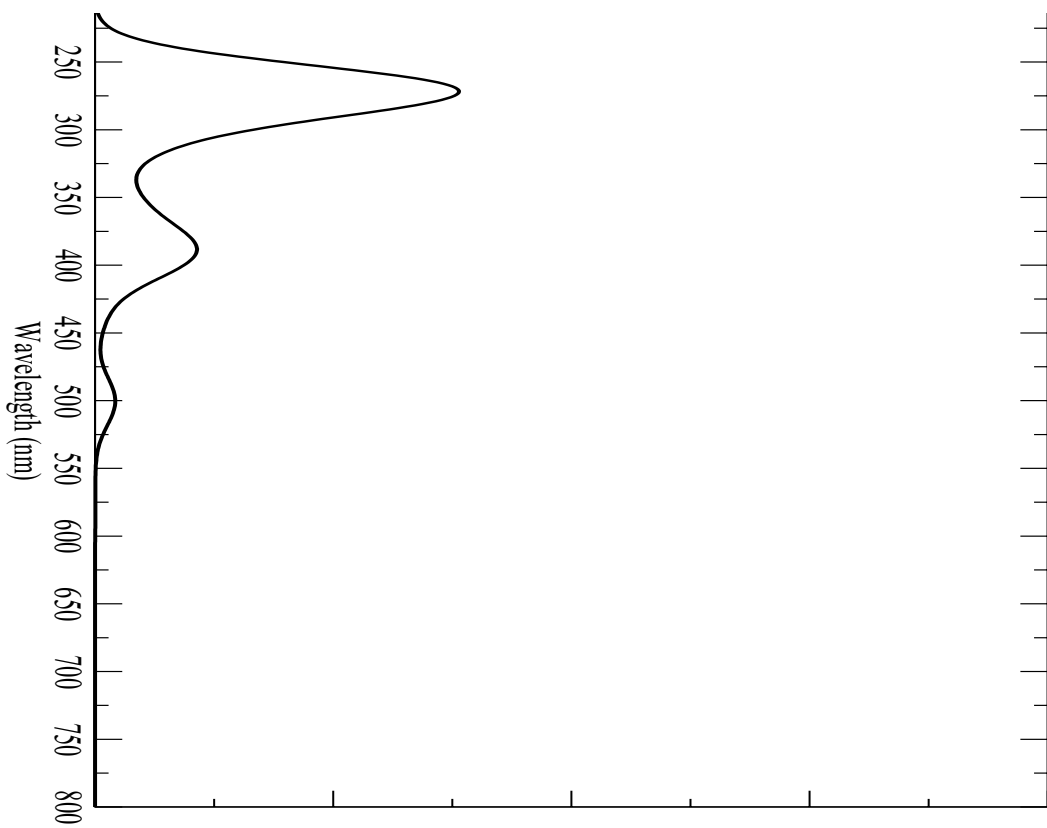
*Figure S5 : spectra of **1-Co***
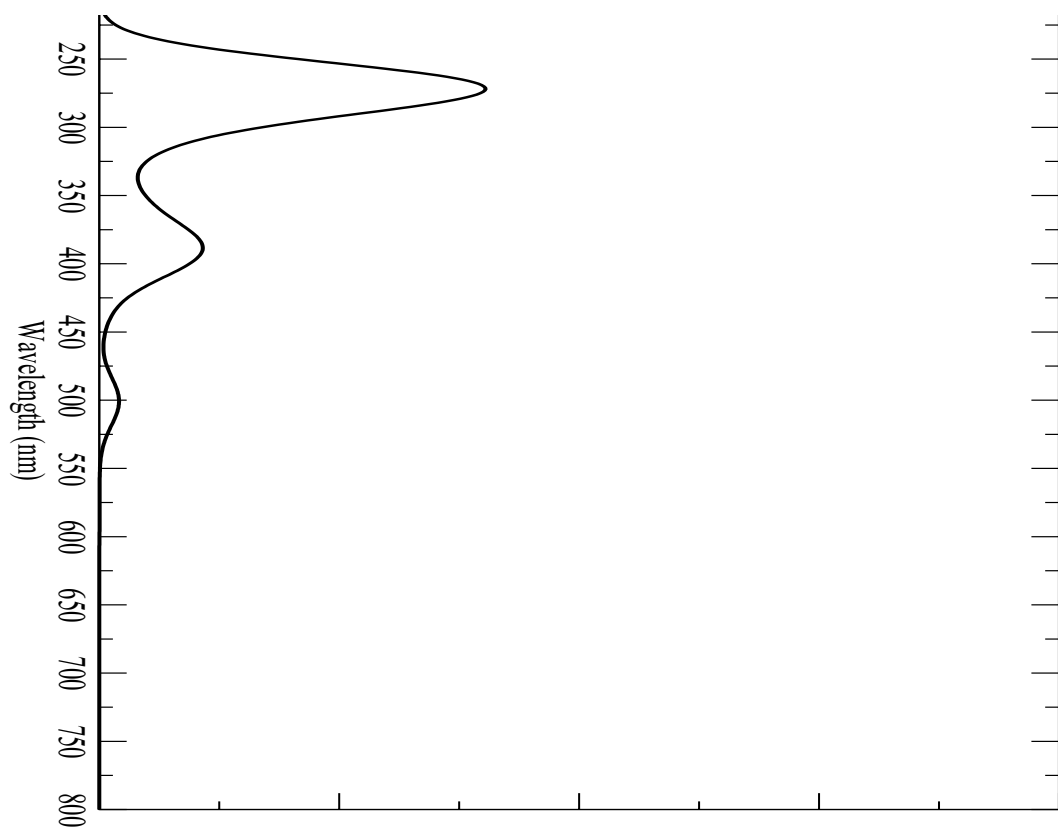
*Figure S6: spectra of **1-Ni***
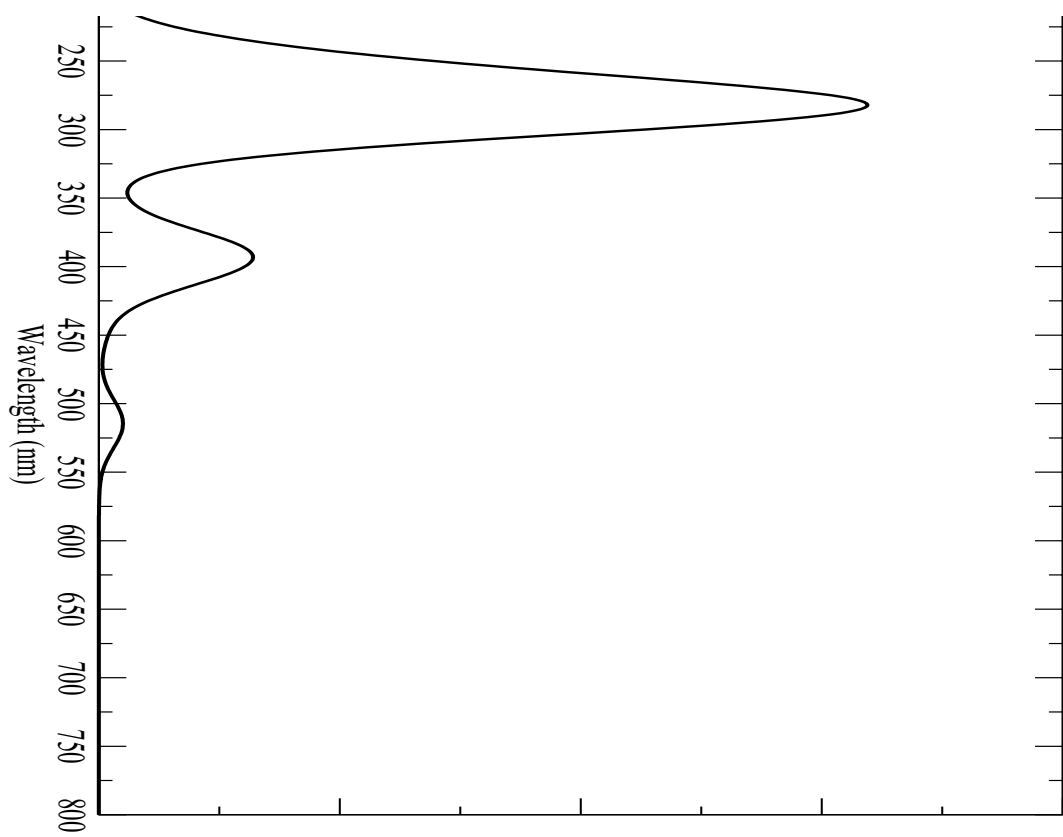
*Figure S7: spectra of **1-Zn***
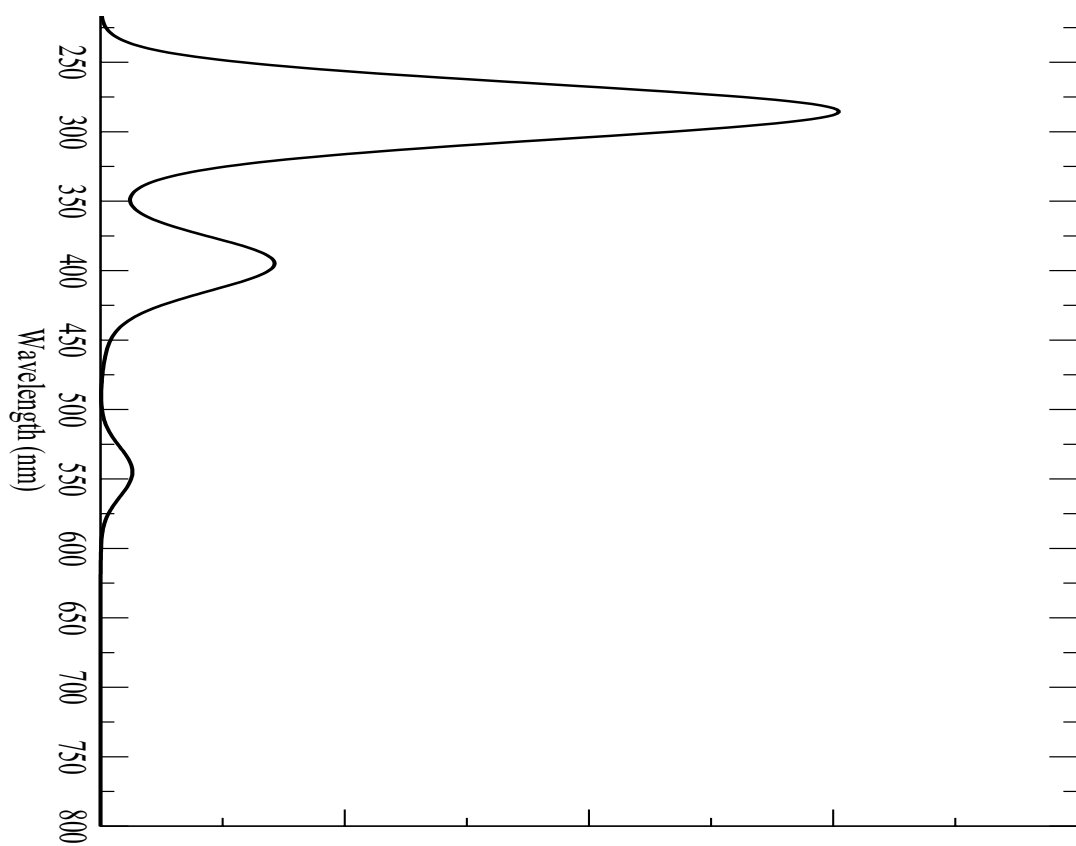
Figure S8: spectra of **1-Rh**
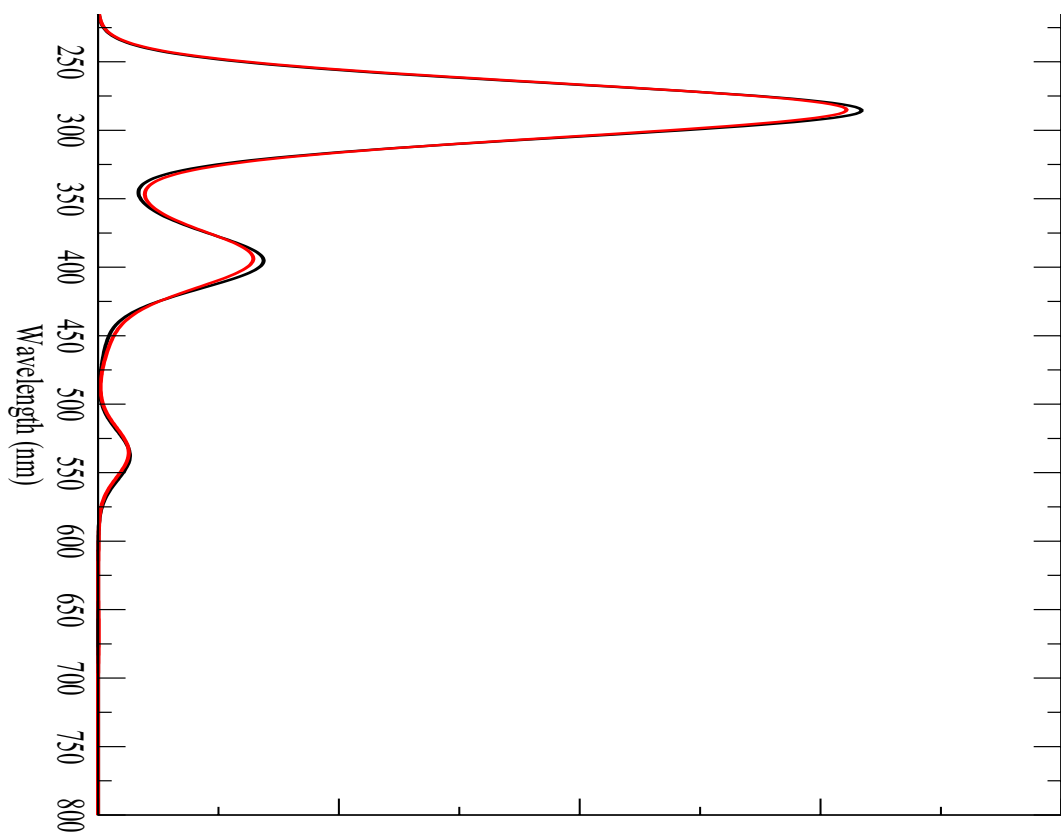
*Figure S9: spectra of **1-Pd**, in black without SOC and in red with SOC*
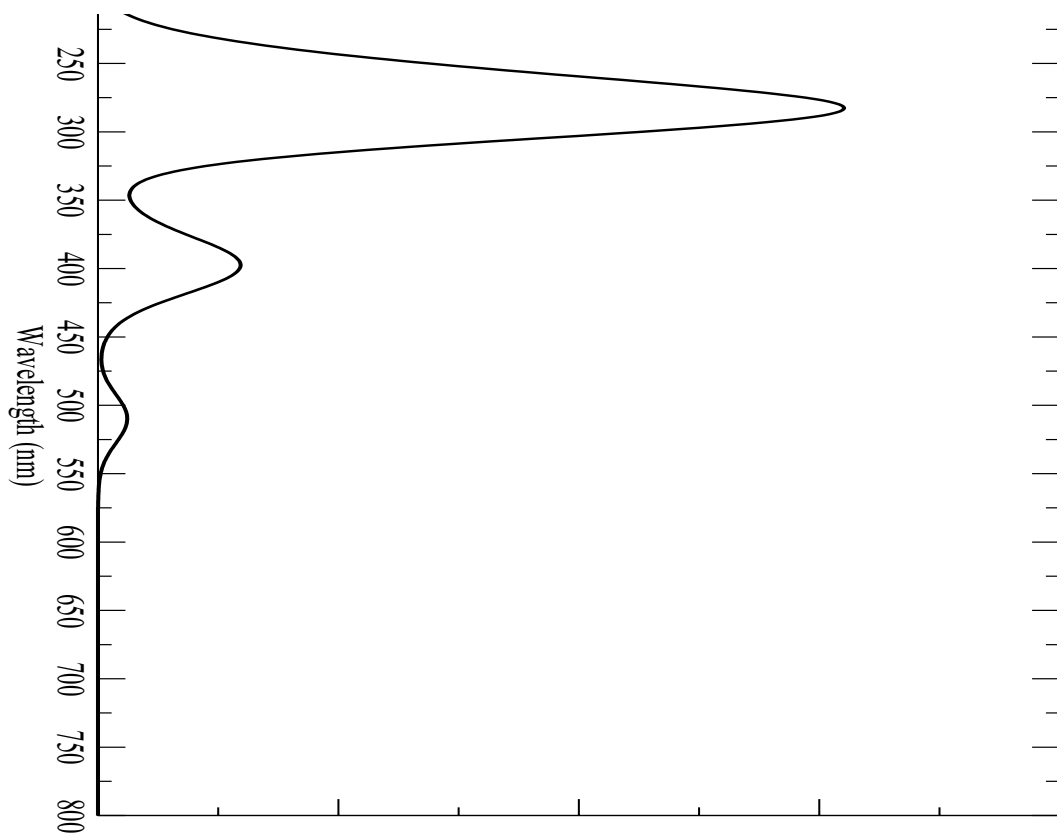
*Figure S10: spectra of **1-Cd***
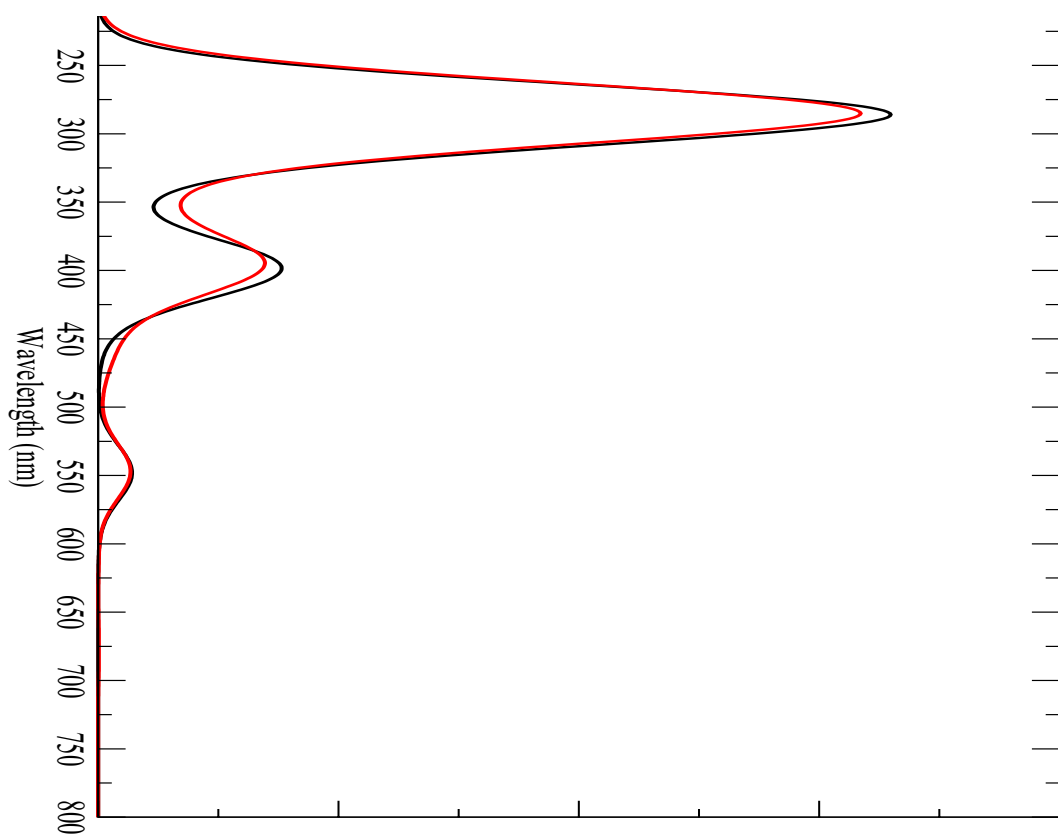
*Figure S11: spectra of **1-Pt**, in black without SOC and in red with SOC*
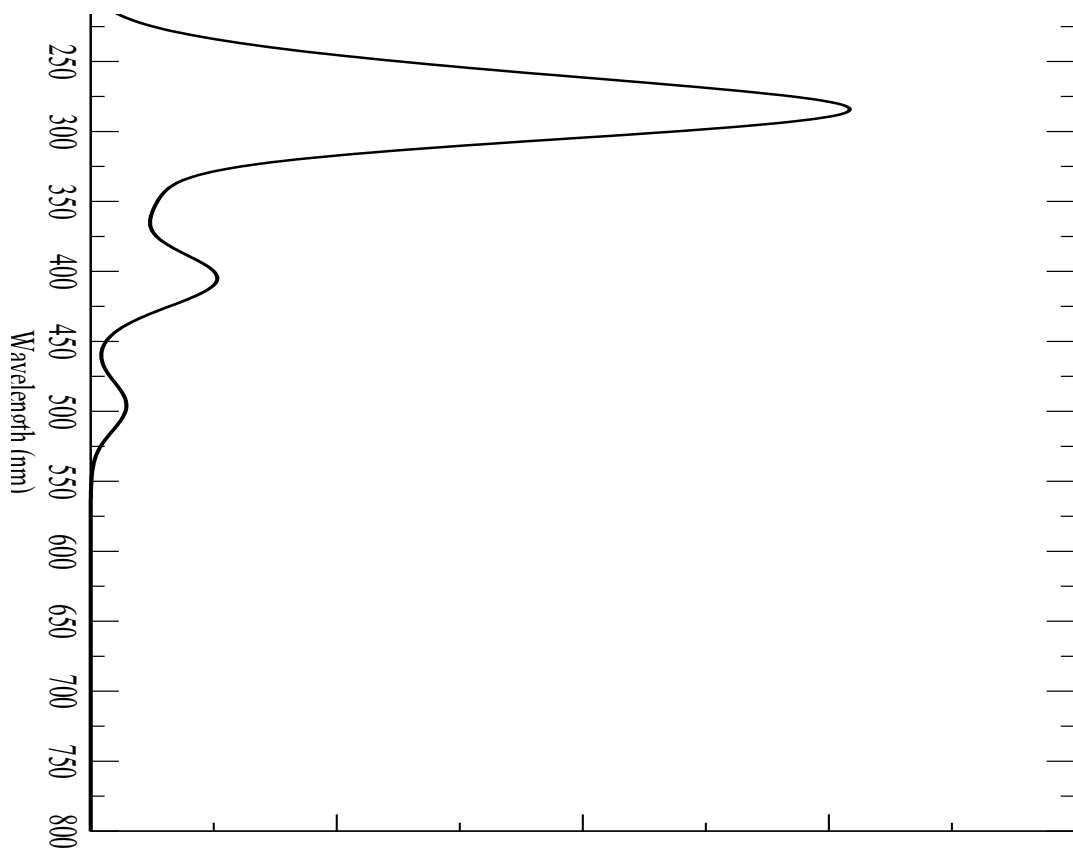
*Figure S12: spectra of **1-Au(I)***
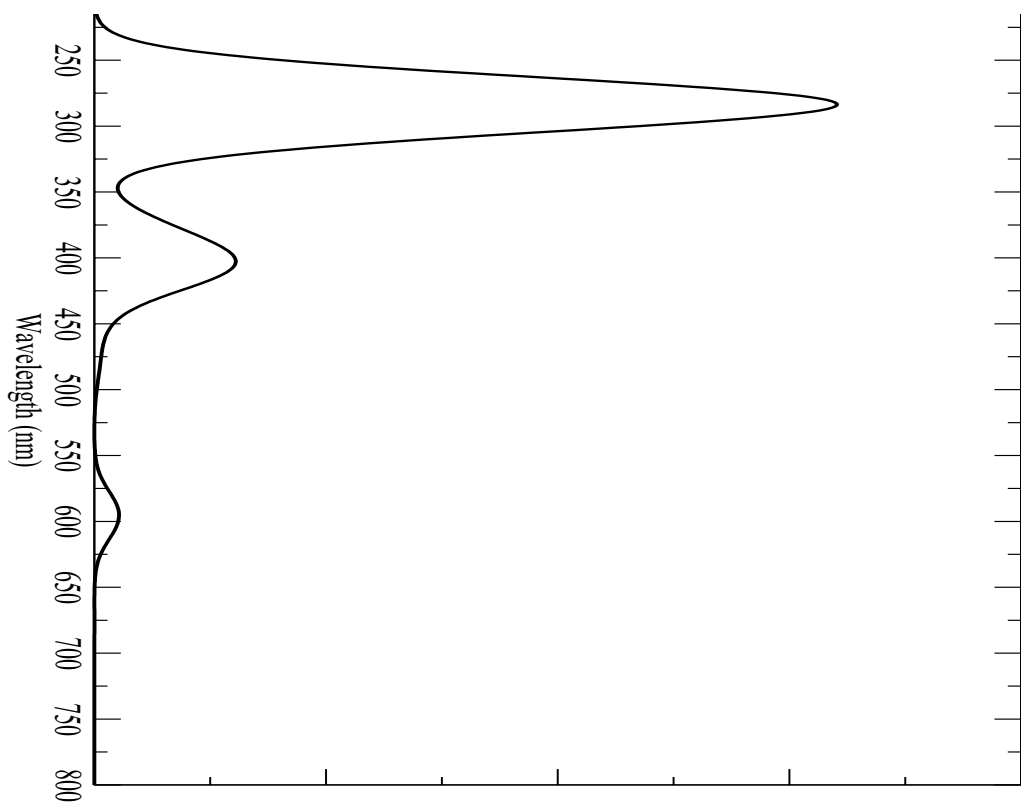
*Figure S13: spectra of **1-Au(III)***
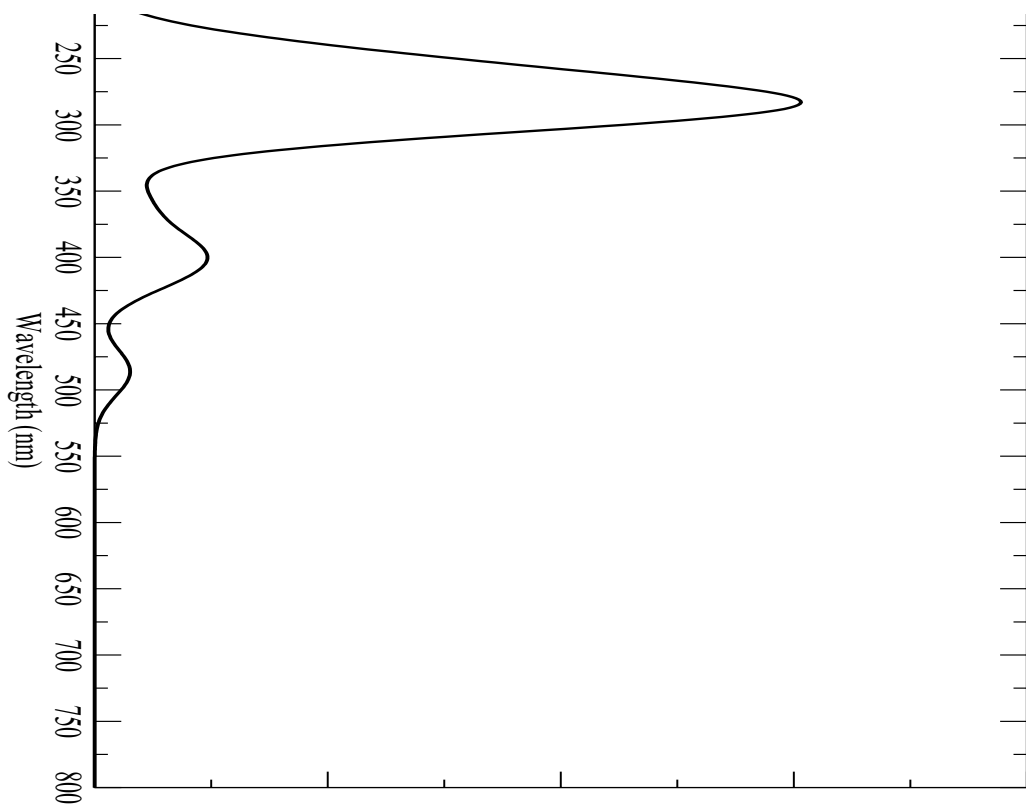
*Figure S14: spectra of **1-Hg***
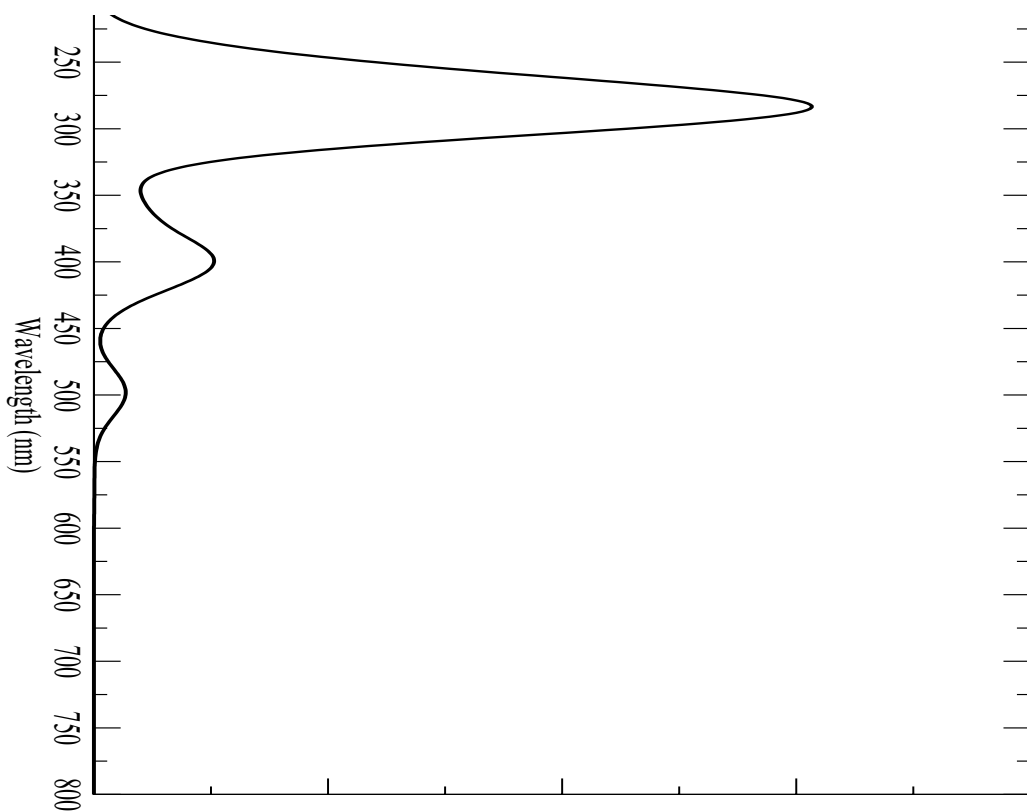
*Figure S15: spectra of **1-Pb***
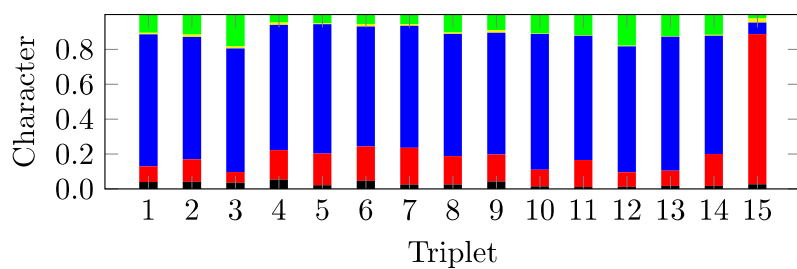
*Figure S16: Character of the low-lying triplet states (T_1-T_{15}) of **1***
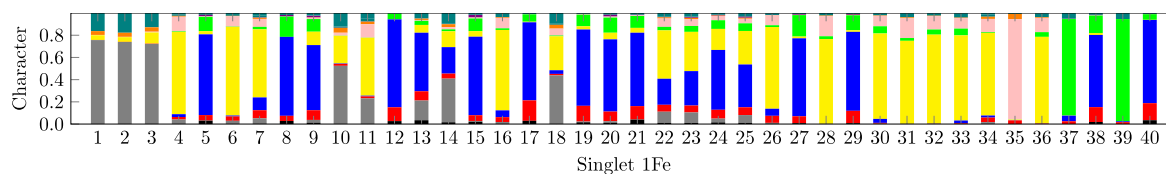
Figure S18: : Character of the low-lying singlet states of 1-Fe
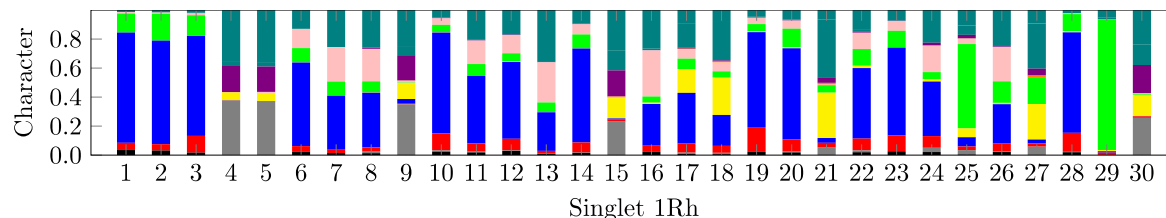
Figure S19: Character of the low-lying singlet states of 1-Rh.
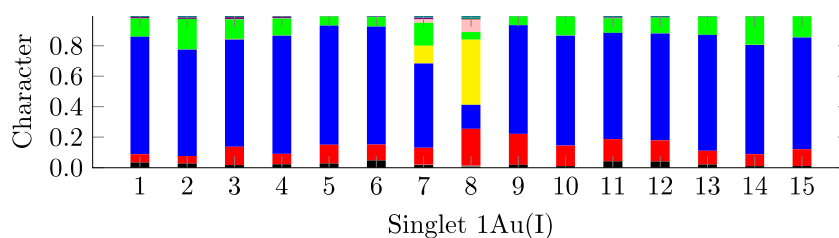
Figure S20 : Character of the low-lying singlet states of 1-Au(I)
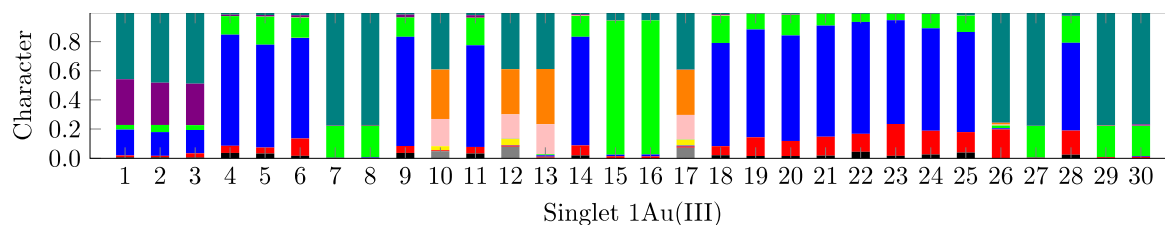
Figure S21 : Character of the low-lying singlet states of 1-Au(III)
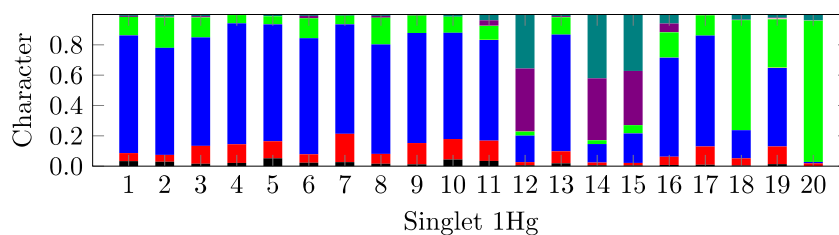
Figure S22 : Character of the low-lying singlet states of 1-Hg

The color code for figures S16 and S17: blue for $M_{Ru}LCT$; green for LLCT; red for LC; black and grey for MC (Ru or Pd); pink for XLCT; yellow for $M_{Pd}LCT$; orange for $XM_{Pd}CT$; violet for $M_{Ru}M_{Pd}CT$; teal for other transitions.

Table S1: Energy (in Ev), oscillator strength and nature of the singlet states of **1**

State	Energy	Oscillator	$M_{Ru}C$	LC	$M_{Ru}LCT$	LLCT	Other
1	2.391	0.00E+00	3.27%	5.75%	78.43%	11.85%	0.70%
2	2.550	3.00E-03	2.79%	5.19%	71.81%	19.30%	0.91%
3	2.686	1.76E-01	1.62%	12.24%	72.90%	12.66%	0.58%
4	2.733	3.00E-03	2.29%	11.96%	79.23%	6.03%	0.50%
5	2.765	5.00E-03	5.09%	11.24%	76.66%	5.91%	1.10%
6	2.880	7.50E-02	2.74%	18.21%	72.24%	5.93%	0.87%
7	2.940	3.00E-03	2.93%	14.73%	71.39%	9.98%	0.97%
8	2.979	2.01E-01	4.19%	14.51%	70.48%	9.50%	1.33%
9	3.104	3.40E-02	1.48%	6.74%	78.88%	12.56%	0.34%
10	3.164	1.18E-01	2.36%	16.20%	72.28%	8.28%	0.88%
11	3.252	1.10E-02	1.40%	6.80%	72.12%	19.21%	0.47%
12	3.318	3.00E-03	1.65%	9.05%	76.47%	12.34%	0.49%
13	3.451	0.00E+00	1.02%	6.88%	73.98%	17.72%	0.39%
14	3.540	1.04E-01	0.99%	11.97%	73.47%	13.23%	0.35%
15	3.567	1.41E-01	1.01%	10.66%	74.68%	13.13%	0.53%
16	3.664	4.00E-03	1.39%	14.00%	77.63%	6.61%	0.37%
17	3.816	4.80E-02	1.71%	19.53%	72.17%	6.11%	0.49%
18	3.838	1.00E-03	2.46%	13.96%	75.66%	7.35%	0.57%
19	3.875	3.30E-02	2.46%	17.07%	69.33%	10.40%	0.75%
20	3.904	1.00E-03	0.05%	3.99%	3.24%	89.90%	2.82%
21	3.943	4.00E-03	13.30%	12.43%	65.71%	5.87%	2.69%
22	3.950	1.20E-02	0.69%	4.82%	2.43%	89.28%	2.78%
23	3.956	4.00E-03	43.71%	5.59%	37.44%	4.53%	8.73%
24	3.964	6.40E-02	6.12%	11.44%	75.20%	5.97%	1.28%
25	3.973	0.00E+00	40.51%	6.66%	40.72%	3.92%	8.20%
26	4.003	4.00E-03	0.92%	22.01%	70.75%	5.79%	0.53%
27	4.010	1.12E-01	4.01%	16.26%	66.25%	12.13%	1.35%
28	4.072	2.00E-02	11.21%	11.48%	64.59%	9.73%	2.99%
29	4.087	1.00E-03	36.54%	8.06%	41.10%	4.88%	9.41%
30	4.102	1.60E-02	8.04%	27.97%	56.32%	4.94%	2.74%
31	4.104	7.00E-03	1.40%	25.28%	62.77%	9.53%	1.03%
32	4.161	1.00E-03	0.06%	90.90%	2.05%	4.16%	2.84%
33	4.234	2.83E-01	0.51%	81.80%	11.74%	3.71%	2.23%
34	4.279	4.57E-01	0.18%	87.51%	6.35%	3.37%	2.58%
35	4.302	1.29E+00	0.53%	81.95%	10.66%	1.97%	4.89%
36	4.332	2.86E-01	0.24%	86.41%	6.04%	2.10%	5.22%
37	4.475	2.20E-02	5.69%	15.50%	61.25%	14.40%	3.17%
38	4.543	1.70E-02	2.95%	11.68%	4.88%	77.39%	3.10%
39	4.562	7.00E-03	18.27%	56.68%	11.84%	6.80%	6.41%
40	4.566	1.00E-03	46.67%	5.95%	29.20%	6.31%	11.86%
41	4.581	2.80E-02	1.82%	21.34%	1.76%	72.23%	2.84%
42	4.591	1.00E-02	29.04%	29.48%	18.43%	14.74%	8.30%
43	4.697	0.00E+00	44.83%	6.69%	30.51%	4.75%	13.22%
44	4.760	1.01E+00	0.09%	87.34%	1.55%	8.02%	2.99%
45	4.798	0.00E+00	0.21%	88.52%	2.48%	6.66%	2.13%
46	4.800	6.00E-03	0.01%	3.74%	0.38%	94.66%	1.22%
47	4.846	4.00E-03	0.02%	3.27%	1.00%	94.51%	1.20%
48	4.927	1.60E-02	0.06%	92.96%	1.72%	3.75%	1.51%
49	4.986	4.00E-03	1.57%	8.46%	73.22%	15.88%	0.86%
50	5.020	6.20E-02	0.03%	8.85%	0.67%	87.70%	2.75%
51	5.050	1.10E-02	0.18%	72.63%	8.75%	17.22%	1.23%
52	5.057	1.00E-03	0.87%	32.00%	53.38%	13.07%	0.68%
53	5.063	1.10E-02	0.12%	18.42%	3.18%	75.59%	2.70%
54	5.076	2.50E-02	0.88%	9.47%	45.59%	41.97%	2.09%
55	5.096	1.60E-02	0.57%	13.72%	20.11%	61.82%	3.78%
56	5.107	5.80E-02	0.01%	83.05%	3.69%	11.80%	1.44%
57	5.128	2.00E-03	0.14%	17.67%	2.79%	74.43%	4.97%
58	5.202	4.30E-02	0.12%	65.80%	22.25%	10.71%	1.12%
59	5.203	0.00E+00	1.19%	51.35%	38.94%	7.27%	1.25%
60	5.227	9.00E-03	0.49%	56.33%	19.54%	21.76%	1.88%
61	5.258	4.20E-02	0.03%	90.26%	4.46%	2.92%	2.34%
62	5.259	0.00E+00	0.05%	23.08%	1.49%	72.94%	2.44%
63	5.279	3.00E-03	0.67%	39.88%	30.67%	27.47%	1.31%
64	5.297	0.00E+00	0.22%	68.34%	14.98%	14.26%	2.21%
65	5.325	2.30E-02	0.29%	32.54%	15.47%	49.19%	2.52%
66	5.333	7.90E-02	0.06%	15.17%	4.01%	78.18%	2.58%
67	5.341	3.60E-02	0.29%	30.02%	57.70%	11.31%	0.69%
68	5.374	2.80E-02	0.76%	37.39%	51.91%	8.65%	1.30%
69	5.395	2.80E-02	0.68%	32.40%	53.67%	12.48%	0.77%
70	5.400	1.00E-03	0.02%	96.15%	1.10%	1.58%	1.15%
71	5.429	2.50E-02	0.11%	78.97%	12.92%	6.96%	1.04%
72	5.452	5.40E-02	0.11%	15.44%	5.91%	75.73%	2.81%
73	5.459	2.00E-03	0.16%	24.18%	31.14%	43.31%	1.21%
74	5.469	7.00E-03	0.15%	21.21%	36.18%	41.48%	0.99%
75	5.485	1.12E-01	0.23%	41.77%	17.80%	38.29%	1.90%
76	5.500	0.00E+00	2.37%	19.58%	49.67%	27.11%	1.27%
77	5.530	2.00E-03	10.75%	14.87%	18.87%	49.73%	5.78%
78	5.542	0.00E+00	15.46%	10.35%	29.70%	38.35%	6.15%
79	5.544	3.00E-03	0.23%	82.15%	1.86%	12.66%	3.10%
80	5.575	1.38E-01	0.85%	35.60%	7.86%	52.91%	2.78%

Table S2: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Ca**

State	Energy	Oscillator	$M_{Ru}C$	$M_{M}C$	LC	$M_{Ru}LCT$	$M_{M}LCT$	LLCT	XLCT	XMCT	$M_{Ru}M_{M}CT$	$M_{M}M_{Ru}CT$	Other
1	2.170	0.00E+00	3.36%	0.00%	5.37%	77.67%	0.03%	12.26%	0.01%	0.00%	0.36%	0.00%	0.95%
2	2.335	2.00E-03	2.83%	0.00%	4.92%	71.57%	0.02%	19.08%	0.01%	0.00%	0.39%	0.00%	1.19%
3	2.503	1.24E-01	1.53%	0.00%	11.56%	71.55%	0.01%	13.76%	0.05%	0.01%	0.53%	0.00%	1.00%
4	2.823	4.00E-03	2.80%	0.00%	12.39%	78.83%	0.02%	5.35%	0.01%	0.00%	0.01%	0.00%	0.60%
5	2.843	3.00E-03	5.02%	0.00%	11.36%	77.15%	0.02%	5.40%	0.01%	0.00%	0.01%	0.00%	1.04%

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
6	2.891	2.40E-02	2.10%	0.00%	5.67%	77.57%	0.03%	12.83%	0.01%	0.00%	0.87%	0.00%	0.94%
7	2.972	5.90E-02	3.15%	0.00%	17.43%	72.11%	0.01%	6.27%	0.01%	0.00%	0.02%	0.00%	1.01%
8	3.016	6.00E-03	1.95%	0.00%	14.29%	72.86%	0.01%	10.17%	0.01%	0.00%	0.06%	0.00%	0.64%
9	3.033	5.70E-02	1.34%	0.00%	8.52%	73.10%	0.01%	15.55%	0.01%	0.00%	0.64%	0.00%	0.84%
10	3.078	1.95E-01	4.32%	0.00%	12.75%	70.12%	0.01%	11.15%	0.01%	0.00%	0.16%	0.00%	1.48%
11	3.105	1.62E-01	2.99%	0.00%	14.45%	70.67%	0.01%	10.11%	0.01%	0.00%	0.47%	0.00%	1.28%
12	3.155	2.80E-02	1.80%	0.00%	7.24%	77.78%	0.02%	12.43%	0.01%	0.00%	0.14%	0.00%	0.59%
13	3.304	3.70E-02	1.06%	0.00%	6.92%	73.66%	0.02%	17.80%	0.01%	0.00%	0.11%	0.00%	0.43%
14	3.368	9.00E-02	0.90%	0.00%	11.84%	72.72%	0.01%	13.98%	0.01%	0.00%	0.13%	0.00%	0.42%
15	3.527	8.00E-03	1.75%	0.00%	13.20%	68.57%	0.01%	15.06%	0.01%	0.00%	0.11%	0.00%	1.29%
16	3.588	5.00E-03	0.14%	0.00%	2.85%	3.79%	0.00%	89.74%	0.01%	0.00%	0.00%	0.00%	3.47%
17	3.632	6.00E-03	0.06%	0.00%	2.33%	1.14%	0.00%	92.88%	0.04%	0.00%	0.00%	0.00%	3.54%
18	3.733	7.00E-03	1.36%	0.00%	15.35%	76.89%	0.02%	5.82%	0.01%	0.00%	0.07%	0.00%	0.48%
19	3.891	3.60E-02	5.26%	0.00%	18.45%	69.94%	0.01%	5.07%	0.01%	0.00%	0.07%	0.00%	1.19%
20	3.913	2.00E-03	11.33%	0.00%	12.16%	66.64%	0.01%	7.45%	0.03%	0.00%	0.06%	0.00%	2.32%
21	3.931	1.00E-02	47.13%	0.00%	5.48%	33.97%	0.01%	3.37%	0.05%	0.00%	0.14%	0.01%	9.84%
22	3.945	4.00E-03	2.04%	0.00%	21.65%	68.51%	0.02%	6.81%	0.03%	0.00%	0.06%	0.00%	0.89%
23	3.954	6.00E-03	0.03%	0.01%	1.31%	0.05%	1.14%	0.12%	93.96%	3.08%	0.00%	0.03%	0.27%
24	3.968	0.00E+00	0.01%	0.01%	1.21%	0.04%	1.05%	0.07%	94.25%	3.08%	0.00%	0.03%	0.26%
25	3.984	3.00E-03	41.78%	0.00%	6.62%	39.20%	0.01%	3.93%	0.02%	0.00%	0.06%	0.00%	8.39%
26	4.013	2.00E-03	0.00%	0.01%	0.71%	0.09%	1.37%	0.05%	94.39%	3.10%	0.00%	0.03%	0.25%
27	4.014	8.00E-03	0.01%	0.01%	0.77%	0.34%	1.51%	0.09%	93.91%	3.08%	0.00%	0.04%	0.24%
28	4.042	3.00E-03	2.17%	0.00%	15.33%	75.61%	0.02%	5.86%	0.40%	0.01%	0.03%	0.00%	0.58%
29	4.055	2.70E-02	11.79%	0.00%	11.82%	67.26%	0.01%	6.03%	0.01%	0.00%	0.04%	0.00%	3.04%
30	4.075	9.90E-02	24.97%	0.00%	9.70%	53.33%	0.01%	5.48%	0.01%	0.00%	0.05%	0.00%	6.45%
31	4.094	5.00E-03	2.68%	0.00%	25.52%	65.69%	0.01%	5.13%	0.01%	0.00%	0.04%	0.00%	0.92%
32	4.099	6.40E-02	14.99%	0.00%	23.34%	48.98%	0.01%	8.14%	0.01%	0.00%	0.07%	0.00%	4.47%
33	4.166	7.70E-02	1.37%	0.00%	37.18%	43.97%	0.01%	16.50%	0.02%	0.00%	0.02%	0.00%	0.95%
34	4.168	8.00E-03	5.41%	0.00%	16.78%	65.58%	0.01%	10.72%	0.02%	0.00%	0.01%	0.00%	1.46%
35	4.172	1.55E-01	2.16%	0.00%	36.16%	53.99%	0.01%	6.47%	0.01%	0.00%	0.02%	0.00%	1.17%
36	4.179	3.00E-03	0.00%	0.03%	0.14%	0.03%	3.92%	0.03%	92.44%	3.06%	0.00%	0.10%	0.23%
37	4.232	1.40E-02	0.62%	0.00%	17.88%	24.87%	0.01%	54.25%	0.01%	0.00%	0.00%	0.00%	2.35%
38	4.262	6.00E-02	0.13%	0.00%	44.64%	7.73%	0.00%	45.29%	0.03%	0.00%	0.01%	0.00%	2.16%
39	4.274	9.50E-02	0.42%	0.00%	59.99%	7.41%	0.00%	27.01%	0.01%	0.00%	0.00%	0.00%	5.16%
40	4.296	1.29E-01	0.24%	0.00%	58.79%	4.53%	0.00%	31.13%	0.02%	0.00%	0.01%	0.00%	5.29%
41	4.337	9.69E-01	0.62%	0.00%	64.62%	20.68%	0.01%	10.02%	0.03%	0.00%	0.01%	0.00%	4.01%
42	4.340	9.11E-01	0.56%	0.00%	64.92%	19.23%	0.01%	11.11%	0.04%	0.00%	0.01%	0.00%	4.14%
43	4.505	1.60E-02	7.11%	0.00%	15.17%	62.01%	0.02%	12.18%	0.10%	0.01%	0.21%	0.00%	3.19%
44	4.520	1.60E-02	0.01%	0.00%	2.45%	0.40%	0.00%	95.66%	0.03%	0.00%	0.00%	0.00%	1.46%
45	4.561	3.00E-03	10.08%	0.06%	5.39%	6.85%	6.11%	3.36%	62.86%	2.15%	0.02%	0.15%	2.95%
46	4.562	3.00E-03	33.40%	0.02%	5.62%	22.71%	1.82%	8.22%	18.67%	0.64%	0.07%	0.05%	8.77%
47	4.565	0.00E+00	4.93%	0.00%	2.72%	4.86%	0.01%	84.82%	0.09%	0.00%	0.02%	0.00%	2.55%
48	4.585	2.00E-03	47.14%	0.00%	4.84%	30.33%	0.13%	4.14%	1.47%	0.05%	0.14%	0.01%	11.75%
49	4.632	6.00E-03	0.08%	0.01%	0.81%	0.08%	1.17%	0.17%	93.72%	3.64%	0.00%	0.03%	0.28%
50	4.641	0.00E+00	0.02%	0.01%	0.90%	0.04%	1.08%	0.12%	93.81%	3.70%	0.00%	0.03%	0.28%
51	4.683	1.10E-02	0.34%	0.01%	2.58%	0.29%	1.29%	0.33%	90.96%	3.73%	0.00%	0.04%	0.42%
52	4.689	9.00E-03	4.89%	0.01%	2.00%	3.55%	1.36%	0.75%	82.44%	3.23%	0.02%	0.04%	1.71%
53	4.691	1.40E-02	33.22%	0.00%	12.93%	23.84%	0.47%	6.14%	12.48%	0.45%	0.11%	0.02%	10.36%
54	4.702	8.74E-01	1.71%	0.01%	81.33%	2.01%	0.21%	8.61%	2.02%	0.06%	0.01%	0.01%	4.04%
55	4.721	6.20E-02	3.61%	0.02%	69.57%	5.25%	2.63%	13.47%	1.26%	0.04%	0.02%	0.07%	4.07%
56	4.842	0.00E+00	0.00%	0.00%	0.09%	0.08%	1.20%	0.79%	94.43%	3.33%	0.00%	0.04%	0.04%
57	4.852	2.00E-03	0.04%	0.04%	0.25%	1.31%	3.79%	0.34%	90.17%	3.68%	0.01%	0.11%	0.26%
58	4.856	0.00E+00	1.41%	0.00%	5.31%	54.65%	0.30%	15.30%	20.55%	0.71%	0.52%	0.01%	1.25%
59	4.856	0.00E+00	0.38%	0.00%	1.34%	13.33%	0.95%	4.10%	76.67%	2.73%	0.13%	0.03%	0.33%
60	4.869	0.00E+00	0.00%	0.00%	0.43%	0.10%	1.24%	0.55%	93.65%	3.92%	0.00%	0.05%	0.05%
61	4.881	0.00E+00	0.00%	0.00%	0.19%	0.02%	1.20%	0.55%	94.05%	3.90%	0.00%	0.05%	0.04%
62	4.895	1.00E-03	0.01%	0.00%	0.57%	0.51%	1.34%	0.62%	94.71%	2.15%	0.00%	0.03%	0.06%
63	4.903	1.00E-03	0.00%	0.00%	0.49%	0.07%	1.20%	0.46%	95.44%	2.26%	0.00%	0.03%	0.05%
64	4.933	5.00E-03	0.01%	0.00%	0.68%	0.75%	1.36%	0.64%	93.26%	3.18%	0.01%	0.05%	0.07%
65	4.936	5.40E-02	0.70%	0.00%	17.89%	49.74%	0.27%	11.42%	17.83%	0.57%	0.40%	0.01%	1.17%
66	4.937	7.00E-03	0.10%	0.00%	2.76%	6.94%	1.16%	2.14%	83.88%	2.71%	0.06%	0.04%	0.21%
67	4.939	0.00E+00	0.07%	0.00%	1.88%	4.35%	1.35%	1.53%	87.70%	2.90%	0.03%	0.04%	0.14%
68	4.946	0.00E+00	0.01%	0.00%	0.30%	0.45%	1.16%	0.89%	93.96%	3.15%	0.00%	0.04%	0.04%
69	4.961	2.30E-02	1.45%	0.00%	10.24%	58.66%	0.10%	24.47%	2.91%	0.14%	0.42%	0.01%	1.60%
70	4.962	3.00E-03	0.28%	0.00%	6.58%	9.40%	0.03%	80.14%	0.34%	0.02%	0.07%	0.00%	3.14%
71	4.979	2.00E-03	0.00%	0.00%	0.29%	0.12%	1.49%	0.74%	94.38%	2.89%	0.00%	0.05%	0.04%
72	4.981	1.00E-03	0.01%	0.00%	0.30%	0.34%	1.36%	1.10%	93.93%	2.87%	0.00%	0.04%	0.06%
73	5.009	5.70E-02	0.08%	0.00%	10.62%	3.45%	0.18%	81.64%	0.60%	0.03%	0.04%	0.01%	3.36%
74	5.042	3.90E-02	0.05%	0.00%	88.75%	2.03%	0.01%	7.79%	0.10%	0.00%	0.00%	0.00%	1.26%
75	5.069	0.00E+00	0.06%	0.00%	4.49%	1.65%	2.69%	25.47%	62.25%	2.13%	0.01%	0.09%	1.16%
76	5.071	1.50E-02	0.15%	0.00%	10.36%	3.93%	1.41%	50.14%	30.62%	1.09%	0.02%	0.05%	2.24%
77	5.087	6.90E-02	0.01%	0.00%	90.75%	2.60%	0.13%	4.68%	0.65%	0.03%	0.00%	0.00%	1.15%
78	5.101	0.00E+00	0.00%	0.01%	1.22%	0.18%	3.71%	3.75%	87.49%	3.30%	0.00%	0.13%	0.20%
79	5.103	1.80E-02	0.11%	0.00%	14.05%	3.81%	0.27%	73.53%	4.76%	0.20%	0.03%	0.01%	3.24%
80	5.143	1.00E-03	0.00%	0.00%	0.11%	0.01%	3.96%	0.11%	93.17%	2.51%	0.00%	0.10%	0.02%

*Table S3: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Mn***

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
1	2.076	6.24E-06											
2	2.155	3.34E-05											
3	2.161	1.46E-03											
4	2.238	4.50E-05											
5	2.304	6.70E-04											
6	2.395	2.24E-03											
7	2.504	8.25E-02											
8	2.719	1.63E-04											
9	2.721	1.37E-05											
10	2.780	5.64E-04											
11	2.785	7.24E-04											
12	2.786	5.71E-04											
13	2.827	9.16E-03											

14	2.838	9.29E-04
15	2.860	1.15E-03
16	2.872	4.21E-05
17	2.879	1.19E-02
18	2.934	4.18E-04
19	2.938	4.13E-04
20	2.956	7.96E-04
21	2.991	1.63E-02
22	3.020	1.56E-02
23	3.025	4.71E-03
24	3.083	7.63E-03
25	3.101	1.71E-03
26	3.117	1.77E-02
27	3.127	1.73E-01
28	3.151	1.04E-01
29	3.196	5.07E-04
30	3.228	7.68E-04
31	3.275	5.48E-02
32	3.325	3.83E-03
33	3.358	6.56E-02
34	3.372	5.34E-03
35	3.373	1.70E-02
36	3.396	2.17E-03
37	3.434	8.36E-04
38	3.458	9.05E-06
39	3.492	6.98E-03
40	3.524	6.53E-04
41	3.535	2.29E-02
42	3.535	2.01E-03
43	3.541	1.33E-02
44	3.565	2.99E-02
45	3.584	8.13E-03
46	3.589	5.59E-03
47	3.607	2.07E-03
48	3.612	6.96E-06
49	3.652	8.64E-04
50	3.677	4.84E-03
51	3.711	7.78E-06
52	3.738	1.41E-04
53	3.742	2.68E-05
54	3.747	1.66E-03
55	3.756	4.00E-04
56	3.761	2.10E-04
57	3.793	1.16E-03
58	3.853	3.02E-03
59	3.891	1.97E-03
60	3.901	1.50E-02
61	3.903	4.17E-04
62	3.913	2.85E-06
63	3.920	1.68E-03
64	3.923	1.31E-03
65	3.927	1.38E-02
66	3.932	2.23E-02
67	3.950	2.27E-05
68	3.953	4.11E-03
69	3.975	6.75E-03
70	3.978	1.55E-03
71	3.979	9.37E-04
72	3.984	2.80E-03
73	3.986	1.54E-03
74	4.013	1.53E-04
75	4.026	4.37E-06
76	4.039	6.68E-05
77	4.051	3.03E-03
78	4.065	3.91E-03
79	4.070	8.16E-04
80	4.087	2.19E-02
81	4.100	1.12E-03
82	4.123	1.93E-03
83	4.125	8.85E-02
84	4.142	7.87E-03
85	4.167	3.37E-03
86	4.174	1.26E-02
87	4.178	1.06E-02
88	4.182	2.91E-03
89	4.189	2.12E-02
90	4.214	6.32E-04
91	4.227	1.78E-03
92	4.235	2.52E-04
93	4.242	2.58E-03
94	4.255	6.53E-04
95	4.279	5.75E-04
96	4.280	7.35E-03
97	4.285	5.58E-05
98	4.289	4.02E-03
99	4.334	3.29E-06
100	4.337	3.00E-03
101	4.350	2.03E-03
102	4.383	2.14E-03
103	4.390	6.53E-03
104	4.420	2.11E-03
105	4.423	3.53E-03
106	4.439	4.29E-03
107	4.445	5.67E-04
108	4.459	2.08E-02
109	4.461	1.23E-03
110	4.469	4.44E-03

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
111	4.490	7.03E-03											
112	4.494	6.64E-03											
113	4.501	1.65E-03											
114	4.504	5.03E-02											
115	4.514	6.93E-02											
116	4.524	2.37E-05											
117	4.535	0.1622											
118	4.541	2.09E-03											
119	4.545	1.93E-02											
120	4.556	2.18E-02											
121	4.557	3.84E-04											
122	4.563	4.18E-03											
123	4.564	3.34E-02											
124	4.575	3.48E-03											
125	4.582	3.35E-02											
126	4.585	4.46E-06											
127	4.598	0.2348											
128	4.612	0.7188											
129	4.615	4.92E-02											
130	4.621	2.25E-02											
131	4.630	9.96E-03											
132	4.656	2.24E-03											
133	4.658	2.12E-02											
134	4.686	1.07E-04											
135	4.688	1.61E-02											
136	4.712	2.65E-08											
137	4.732	2.44E-03											
138	4.749	7.21E-04											
139	4.762	0.101											
140	4.774	1.67E-04											
141	4.792	5.49E-02											
142	4.802	3.81E-04											
143	4.815	6.92E-06											
144	4.829	6.00E-04											
145	4.833	0.1086											
146	4.842	5.57E-03											
147	4.848	6.26E-05											
148	4.858	1.47E-04											
149	4.864	1.94E-03											
150	4.880	1.29E-02											
151	4.881	2.81E-02											
152	4.888	8.08E-04											
153	4.890	1.94E-04											
154	4.901	3.82E-03											
155	4.909	3.68E-02											
156	4.910	1.87E-02											
157	4.920	1.93E-03											
158	4.941	1.12E-04											
159	4.950	1.36E-03											
160	4.959	4.42E-04											

*Table S4: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Fe***

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
1	1.684	0.00E+00	0.00%	70.89%	0.17%	0.00%	3.57%	0.00%	0.24%	4.88%	0.01%	0.03%	20.21%
2	1.792	0.00E+00	0.00%	68.91%	0.24%	0.00%	3.87%	0.00%	0.26%	4.78%	0.01%	0.04%	21.89%
3	1.958	0.00E+00	0.00%	3.19%	3.50%	0.01%	75.56%	0.06%	14.35%	0.78%	0.00%	1.37%	1.19%
4	2.121	0.00E+00	1.60%	3.11%	3.41%	39.06%	41.27%	6.40%	2.03%	0.19%	0.70%	0.69%	1.54%
5	2.146	0.00E+00	0.10%	73.52%	0.42%	2.13%	11.24%	0.34%	0.48%	2.40%	0.06%	0.24%	9.09%
6	2.161	0.00E+00	1.52%	5.11%	3.97%	36.08%	42.21%	5.61%	2.17%	0.27%	0.62%	0.68%	1.77%
7	2.165	6.50E-02	0.10%	5.01%	6.46%	4.12%	62.76%	0.82%	15.16%	1.20%	0.11%	1.91%	2.36%
8	2.308	2.00E-03	2.74%	0.06%	4.54%	70.89%	0.56%	18.05%	0.04%	0.01%	1.27%	0.01%	1.84%
9	2.485	8.80E-02	1.47%	1.99%	9.41%	65.68%	3.39%	12.53%	1.24%	0.14%	1.69%	0.08%	2.39%
10	2.625	0.00E+00	0.02%	50.44%	1.69%	0.90%	23.45%	0.22%	5.06%	2.26%	0.06%	0.95%	14.95%
11	2.776	1.40E-02	0.03%	2.13%	3.41%	1.31%	73.01%	0.32%	15.11%	0.99%	0.04%	2.78%	0.86%
12	2.831	4.00E-03	2.77%	0.00%	12.60%	78.84%	0.16%	4.98%	0.03%	0.00%	0.03%	0.01%	0.59%
13	2.850	3.00E-03	5.08%	0.00%	11.57%	77.06%	0.12%	5.05%	0.03%	0.00%	0.03%	0.01%	1.05%
14	2.896	1.00E-03	0.09%	23.19%	1.89%	3.71%	57.77%	0.74%	3.16%	2.15%	0.17%	2.74%	4.41%
15	2.959	6.00E-03	1.66%	2.23%	5.38%	61.99%	10.43%	10.98%	2.05%	0.25%	2.57%	0.23%	2.22%
16	2.993	2.90E-02	3.05%	0.02%	17.56%	69.27%	1.87%	6.58%	0.45%	0.05%	0.08%	0.08%	1.06%
17	3.004	1.00E-03	0.17%	15.53%	5.21%	10.45%	48.11%	1.86%	11.63%	1.21%	0.06%	0.80%	4.98%
18	3.022	1.00E-03	1.94%	4.91%	11.51%	55.36%	13.08%	7.40%	2.79%	0.50%	0.08%	0.48%	1.96%
19	3.026	8.80E-02	0.23%	1.22%	6.63%	13.75%	59.18%	2.92%	13.59%	0.45%	0.46%	0.92%	0.66%
20	3.042	1.00E-03	0.14%	39.80%	2.29%	5.79%	36.37%	0.79%	2.10%	3.74%	0.02%	0.61%	8.34%
21	3.067	2.02E-01	2.84%	0.08%	14.73%	66.87%	4.65%	8.34%	1.10%	0.03%	0.22%	0.08%	1.06%
22	3.123	5.30E-02	2.31%	1.66%	5.54%	63.85%	5.10%	15.20%	1.15%	0.20%	2.36%	0.15%	2.50%
23	3.128	1.58E-01	2.14%	1.34%	9.28%	70.37%	3.42%	10.11%	0.94%	0.25%	0.74%	0.15%	1.26%
24	3.154	7.30E-02	1.96%	0.47%	10.28%	70.55%	1.16%	11.34%	0.31%	0.07%	1.96%	0.02%	1.88%
25	3.158	2.00E-03	0.09%	21.28%	0.99%	2.58%	54.93%	2.50%	9.02%	2.41%	0.10%	1.84%	4.26%
26	3.194	0.00E+00	0.01%	21.06%	0.58%	0.37%	56.92%	2.31%	10.79%	2.30%	0.02%	1.56%	4.08%
27	3.210	2.00E-02	0.10%	0.30%	1.23%	4.50%	68.52%	5.50%	17.38%	0.57%	0.02%	1.56%	0.32%
28	3.228	8.00E-03	0.01%	0.24%	0.36%	0.59%	71.82%	3.51%	18.06%	1.15%	0.01%	3.85%	0.41%
29	3.253	6.90E-02	0.24%	3.89%	3.29%	16.38%	50.09%	4.89%	15.68%	2.00%	0.27%	1.05%	2.22%
30	3.266	3.00E-03	0.08%	21.24%	2.60%	2.78%	58.25%	0.55%	6.20%	2.53%	0.03%	0.86%	4.88%
31	3.267	1.30E-02	0.27%	0.04%	1.05%	4.04%	66.47%	5.90%	17.72%	0.87%	0.01%	3.25%	0.38%
32	3.300	7.00E-02	0.85%	1.68%	6.09%	57.12%	14.09%	13.88%	3.55%	0.52%	0.69%	0.33%	1.21%
33	3.342	8.60E-02	0.92%	0.01%	10.71%	72.17%	0.50%	13.63%	0.27%	0.02%	1.01%	0.03%	0.76%
34	3.451	0.00E+00	0.01%	0.04%	0.12%	0.15%	89.02%	2.72%	5.03%	0.15%	0.00%	2.66%	0.10%
35	3.503	5.00E-03	0.10%	0.01%	0.51%	3.03%	83.65%	3.34%	4.73%	0.24%	0.03%	4.15%	0.22%
36	3.528	3.90E-02	1.13%	0.01%	8.70%	41.68%	3.50%	41.35%	0.31%	0.01%	0.34%	0.17%	2.81%
37	3.550	3.00E-02	0.86%	0.00%	6.64%	26.86%	0.65%	60.70%	0.10%	0.01%	0.15%	0.03%	3.99%
38	3.584	5.00E-03	0.05%	0.00%	1.95%	0.89%	0.01%	91.20%	0.42%	0.02%	0.02%	0.00%	5.45%

39	3.739	6.00E-03	3.75%	0.00%	15.24%	74.62%	0.18%	5.02%	0.07%	0.00%	0.16%	0.01%	0.95%
40	3.845	0.00E+00	0.11%	0.02%	2.25%	0.22%	0.57%	0.57%	90.47%	4.78%	0.01%	0.01%	1.00%
41	3.853	0.00E+00	0.03%	0.03%	1.78%	0.05%	0.60%	0.08%	91.71%	4.80%	0.00%	0.02%	0.91%
42	3.858	1.00E-03	46.61%	0.00%	4.69%	34.01%	0.04%	3.31%	0.33%	0.02%	0.98%	0.04%	9.96%
43	3.894	2.00E-03	21.12%	0.01%	9.09%	55.48%	2.91%	6.25%	0.73%	0.02%	0.19%	0.05%	4.15%
44	3.918	4.00E-02	4.52%	0.00%	19.49%	69.52%	0.39%	4.60%	0.18%	0.00%	0.14%	0.01%	1.16%
45	3.950	3.00E-03	1.40%	0.01%	20.56%	66.39%	3.76%	5.98%	0.97%	0.02%	0.08%	0.05%	0.78%
46	3.966	4.00E-03	32.33%	0.01%	6.71%	41.55%	5.99%	4.85%	1.52%	0.03%	0.27%	0.08%	6.66%
47	3.992	9.00E-03	0.02%	0.21%	3.88%	0.10%	51.91%	2.31%	38.81%	1.95%	0.00%	0.32%	0.49%
48	4.007	3.20E-02	0.66%	0.10%	6.39%	0.69%	33.72%	1.81%	52.41%	2.13%	0.01%	0.93%	1.15%
49	4.023	5.00E-03	43.62%	0.00%	5.18%	33.59%	0.93%	4.21%	0.93%	0.05%	0.54%	0.04%	10.92%
50	4.037	2.70E-02	0.33%	0.20%	6.45%	4.08%	29.36%	2.63%	52.83%	2.31%	0.00%	0.76%	1.04%
51	4.042	1.70E-02	1.27%	0.28%	8.73%	25.54%	30.70%	4.08%	26.82%	1.54%	0.02%	0.19%	0.84%
52	4.063	0.00E+00	1.58%	0.10%	12.84%	58.04%	12.24%	5.08%	8.86%	0.50%	0.05%	0.09%	0.61%
53	4.068	8.40E-02	4.21%	0.00%	13.30%	75.21%	0.62%	5.34%	0.19%	0.01%	0.05%	0.01%	1.08%
54	4.087	8.60E-02	4.31%	0.02%	19.26%	54.15%	9.26%	8.86%	2.26%	0.04%	0.11%	0.15%	1.60%
55	4.111	7.00E-03	2.07%	0.00%	26.39%	65.26%	0.42%	4.69%	0.21%	0.01%	0.06%	0.01%	0.90%
56	4.160	4.00E-03	0.02%	0.09%	1.43%	1.04%	73.97%	3.90%	17.96%	0.30%	0.00%	1.12%	0.17%
57	4.164	1.80E-02	5.74%	0.00%	12.58%	65.77%	3.55%	9.76%	0.87%	0.03%	0.12%	0.10%	1.48%
58	4.171	1.86E-01	0.42%	0.03%	41.62%	32.61%	14.67%	5.24%	3.77%	0.07%	0.01%	0.23%	1.34%
59	4.172	7.70E-02	1.23%	0.01%	36.22%	46.24%	4.31%	9.73%	1.01%	0.02%	0.03%	0.06%	1.14%
60	4.209	2.60E-02	0.36%	0.05%	7.50%	26.46%	46.26%	5.76%	12.48%	0.20%	0.02%	0.67%	0.23%
61	4.251	7.90E-02	0.68%	0.00%	47.90%	22.08%	1.96%	24.74%	0.48%	0.00%	0.01%	0.01%	2.13%
62	4.271	0.00E+00	0.02%	0.05%	0.24%	0.39%	90.15%	2.78%	5.09%	0.07%	0.00%	1.14%	0.08%
63	4.273	1.70E-02	0.02%	0.00%	80.79%	3.53%	0.17%	12.19%	0.09%	0.00%	0.01%	0.00%	3.20%
64	4.294	1.20E-02	0.10%	0.00%	34.66%	1.49%	0.11%	56.46%	0.05%	0.00%	0.01%	0.00%	7.13%
65	4.311	5.39E-01	0.54%	0.00%	33.09%	16.89%	1.14%	43.17%	0.43%	0.02%	0.02%	0.03%	4.67%
66	4.330	3.77E-01	0.47%	0.00%	58.98%	11.89%	12.05%	9.43%	3.06%	0.04%	0.01%	0.13%	3.95%
67	4.334	3.30E-02	0.03%	0.00%	3.81%	0.82%	71.42%	3.90%	17.40%	0.45%	0.01%	1.83%	0.33%
68	4.341	6.39E-01	0.23%	0.00%	25.70%	10.76%	26.01%	26.98%	6.39%	0.04%	0.01%	0.15%	3.74%
69	4.344	3.26E-01	0.14%	0.00%	12.92%	6.48%	52.53%	13.28%	12.63%	0.08%	0.01%	0.31%	1.63%
70	4.370	4.00E-02	0.90%	0.01%	1.99%	4.47%	66.75%	6.11%	17.16%	0.43%	0.03%	1.70%	0.45%
71	4.382	5.40E-02	0.80%	0.01%	7.43%	8.94%	59.68%	5.98%	16.16%	0.07%	0.03%	0.33%	0.58%
72	4.401	7.00E-03	0.05%	0.33%	0.97%	0.54%	9.80%	0.32%	82.27%	4.46%	0.04%	0.21%	1.01%
73	4.435	0.00E+00	0.02%	0.10%	0.13%	0.23%	90.06%	2.80%	5.09%	0.08%	0.00%	1.37%	0.11%
74	4.481	2.30E-02	0.04%	0.00%	2.47%	0.42%	94.07%	0.05%	0.00%	0.01%	0.00%	2.92%	
75	4.492	2.00E-03	28.00%	0.01%	7.54%	36.18%	1.61%	14.95%	0.84%	0.05%	1.94%	0.05%	8.83%
76	4.512	6.00E-03	12.66%	0.01%	4.38%	16.35%	0.34%	34.83%	0.36%	0.03%	16.47%	0.03%	14.54%
77	4.526	4.00E-03	2.12%	0.01%	4.71%	15.68%	0.79%	52.14%	0.63%	0.04%	13.23%	0.02%	10.64%
78	4.529	2.00E-03	43.23%	0.00%	4.91%	29.86%	0.45%	3.98%	0.16%	0.03%	4.20%	0.05%	13.15%
79	4.557	3.00E-03	12.55%	0.01%	5.36%	23.88%	1.98%	3.63%	0.36%	0.04%	30.22%	0.07%	21.92%
80	4.609	2.00E-03	0.44%	0.00%	0.56%	1.44%	86.83%	2.88%	4.93%	0.13%	0.20%	2.25%	0.35%

*Table S5: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Co***

State	Energy	Oscillator	$M_{Ru}C$	$M_M C$	LC	$M_{Ru}LCT$	$M_M LCT$	LLCT	XLCT	XMCT	$M_{Ru}M_M CT$	$M_M M_{Ru}CT$	Other
1	0.247	2.89E-09											
2	0.268	6.43E-06											
3	1.467	8.94E-06											
4	1.476	8.58E-07											
5	2.035	1.91E-05											
6	2.115	4.95E-06											
7	2.127	1.70E-03											
8	2.211	4.09E-05											
9	2.281	7.95E-04											
10	2.380	1.52E-06											
11	2.397	1.22E-05											
12	2.478	8.51E-02											
13	2.725	4.45E-05											
14	2.729	2.77E-04											
15	2.783	4.42E-03											
16	2.796	2.13E-04											
17	2.797	3.99E-04											
18	2.801	4.05E-03											
19	2.815	4.09E-03											
20	2.848	5.24E-03											
21	2.853	2.51E-03											
22	2.867	2.06E-03											
23	2.881	3.06E-03											
24	2.891	1.09E-02											
25	2.954	1.36E-03											
26	2.961	1.08E-04											
27	2.962	1.15E-03											
28	2.977	2.07E-04											
29	3.008	1.12E-02											
30	3.048	3.46E-03											
31	3.048	1.02E-02											
32	3.066	2.99E-04											
33	3.087	6.17E-05											
34	3.107	5.09E-05											
35	3.110	3.58E-05											
36	3.145	1.82E-01											
37	3.155	1.19E-01											
38	3.179	1.16E-03											
39	3.222	5.35E-04											
40	3.277	7.59E-02											
41	3.340	5.59E-02											
42	3.354	4.71E-03											
43	3.364	4.29E-03											
44	3.375	1.74E-02											
45	3.448	8.81E-06											
46	3.490	2.64E-04											

47	3.506	5.93E-04
48	3.511	4.49E-05
49	3.524	3.44E-03
50	3.527	6.32E-03
51	3.529	9.43E-03
52	3.541	3.00E-05
53	3.552	5.85E-03
54	3.555	4.63E-03
55	3.556	2.66E-02
56	3.560	4.12E-02
57	3.580	2.16E-06
58	3.606	2.03E-03
59	3.679	3.31E-05
60	3.691	4.44E-03
61	3.698	9.70E-04
62	3.723	2.70E-04
63	3.729	1.41E-05
64	3.735	2.84E-04
65	3.737	7.71E-04
66	3.739	2.62E-04
67	3.741	3.26E-05
68	3.741	1.25E-06
69	3.758	1.08E-03
70	3.770	7.84E-05
71	3.774	2.28E-03
72	3.780	1.82E-04
73	3.812	1.01E-03
74	3.828	2.51E-04
75	3.831	6.04E-06
76	3.840	3.21E-05
77	3.853	9.27E-05
78	3.871	3.15E-03
79	3.908	3.30E-04
80	3.915	1.31E-04
81	3.918	6.97E-04
82	3.921	4.81E-05
83	3.936	7.37E-03
84	3.939	2.65E-02
85	3.942	4.87E-04
86	3.949	2.31E-02
87	3.960	1.08E-04
88	3.967	8.33E-05
89	3.968	1.88E-03
90	3.970	2.26E-04
91	3.988	6.89E-03
92	3.997	2.13E-05
93	4.000	1.63E-03
94	4.015	6.25E-04
95	4.038	1.06E-04
96	4.039	9.11E-03
97	4.073	2.56E-03
98	4.080	4.34E-03
99	4.081	1.05E-03
100	4.086	7.05E-04
101	4.105	3.28E-02
102	4.124	2.27E-03
103	4.128	9.31E-07
104	4.134	1.58E-03
105	4.143	8.49E-02
106	4.159	6.96E-04
107	4.168	3.31E-03
108	4.172	6.78E-07
109	4.183	3.16E-03
110	4.184	5.27E-03
111	4.190	9.43E-03
112	4.193	1.50E-03
113	4.203	1.17E-04
114	4.206	2.60E-02
115	4.225	6.95E-03
116	4.230	1.42E-02
117	4.236	3.68E-03
118	4.236	1.55E-03
119	4.237	7.09E-05
120	4.243	4.85E-03
121	4.267	3.20E-03
122	4.273	6.94E-05
123	4.276	3.33E-03
124	4.279	8.98E-05
125	4.282	5.23E-03
126	4.330	1.43E-04
127	4.337	1.88E-03
128	4.344	1.79E-03
129	4.371	1.46E-03
130	4.408	2.70E-04
131	4.414	6.63E-04
132	4.426	7.78E-03
133	4.431	5.28E-03
134	4.441	2.02E-03
135	4.445	4.01E-06
136	4.454	5.14E-04
137	4.457	6.79E-06
138	4.464	3.80E-03
139	4.466	1.09E-03
140	4.471	3.63E-02
141	4.478	1.89E-03
142	4.502	1.96E-02
143	4.522	2.85E-02

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
144	4.533	1.53E-01											
145	4.540	2.33E-04											
146	4.545	6.87E-03											
147	4.551	1.10E-01											
148	4.556	2.08E-05											
149	4.567	2.78E-03											
150	4.571	6.56E-02											
151	4.591	1.61E-02											
152	4.598	6.20E-02											
153	4.609	4.59E-05											
154	4.615	9.01E-01											
155	4.632	1.10E-04											
156	4.659	1.28E-03											
157	4.674	2.43E-03											
158	4.678	2.79E-02											
159	4.714	1.20E-03											
160	4.731	7.74E-05											

*Table S6: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Ni***

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
1	1.740	9.20E-09											
2	1.768	1.50E-07											
3	1.958	2.10E-05											
4	2.035	1.44E-05											
5	2.115	6.49E-06											
6	2.123	1.75E-03											
7	2.208	4.00E-05											
8	2.279	8.72E-04											
9	2.476	8.24E-02											
10	2.521	2.82E-05											
11	2.530	7.33E-05											
12	2.564	3.43E-06											
13	2.731	2.79E-04											
14	2.732	8.82E-03											
15	2.802	4.94E-03											
16	2.802	4.31E-05											
17	2.850	6.80E-03											
18	2.857	9.92E-04											
19	2.874	2.82E-03											
20	2.885	2.80E-03											
21	2.893	1.05E-02											
22	2.953	1.22E-03											
23	2.963	2.04E-03											
24	2.978	4.86E-04											
25	3.010	1.06E-02											
26	3.026	5.86E-03											
27	3.048	3.02E-03											
28	3.051	9.79E-03											
29	3.067	4.37E-04											
30	3.110	3.71E-04											
31	3.148	1.84E-01											
32	3.155	1.15E-01											
33	3.178	1.19E-03											
34	3.221	9.98E-04											
35	3.279	7.75E-02											
36	3.338	5.55E-02											
37	3.349	2.91E-03											
38	3.363	4.48E-03											
39	3.373	2.05E-02											
40	3.395	7.92E-04											
41	3.404	2.04E-04											
42	3.442	1.55E-05											
43	3.494	3.94E-04											
44	3.496	6.65E-05											
45	3.524	5.62E-03											
46	3.534	4.22E-03											
47	3.548	4.99E-03											
48	3.558	6.43E-02											
49	3.572	3.73E-06											
50	3.587	8.46E-04											
51	3.600	6.10E-03											
52	3.608	1.33E-04											
53	3.627	2.31E-03											
54	3.669	4.11E-05											
55	3.692	5.34E-03											
56	3.702	2.97E-04											
57	3.717	7.43E-04											
58	3.743	2.74E-05											
59	3.745	1.52E-04											
60	3.758	5.25E-05											
61	3.761	1.70E-03											
62	3.765	1.43E-04											
63	3.766	2.72E-03											
64	3.785	3.27E-04											
65	3.796	9.58E-05											
66	3.814	1.06E-03											
67	3.839	2.25E-04											
68	3.872	3.01E-03											
69	3.882	2.63E-07											
70	3.917	4.21E-04											
71	3.922	1.43E-04											

72	3.940	2.71E-02
73	3.949	2.28E-02
74	3.960	1.67E-05
75	3.966	6.36E-05
76	3.968	1.24E-03
77	3.986	6.14E-03
78	3.996	2.82E-04
79	4.001	2.20E-03
80	4.043	2.58E-05
81	4.057	5.77E-04
82	4.075	2.75E-03
83	4.085	2.07E-03
84	4.103	2.73E-02
85	4.114	8.15E-04
86	4.117	5.05E-05
87	4.124	5.61E-03
88	4.133	9.45E-04
89	4.138	7.31E-05
90	4.142	9.72E-02
91	4.147	5.08E-03
92	4.158	1.20E-03
93	4.169	3.22E-03
94	4.172	5.41E-03
95	4.182	3.60E-03
96	4.184	4.69E-03
97	4.191	1.36E-03
98	4.202	2.15E-05
99	4.206	1.76E-02
100	4.214	1.49E-05
101	4.222	1.16E-02
102	4.225	6.41E-03
103	4.237	3.77E-03
104	4.276	1.53E-04
105	4.279	4.75E-03
106	4.281	1.45E-05
107	4.285	4.86E-03
108	4.295	1.23E-04
109	4.315	1.64E-03
110	4.332	2.51E-03
111	4.337	5.80E-05
112	4.342	2.39E-04
113	4.344	3.84E-03
114	4.349	1.09E-03
115	4.367	3.03E-04
116	4.370	1.14E-04
117	4.374	2.24E-03
118	4.379	2.08E-02
119	4.407	1.30E-03
120	4.426	4.60E-03
121	4.431	6.25E-03
122	4.442	7.66E-04
123	4.446	1.39E-05
124	4.459	5.22E-03
125	4.460	1.68E-04
126	4.464	6.01E-03
127	4.466	1.93E-03
128	4.468	6.59E-06
129	4.470	3.38E-02
130	4.501	5.97E-04
131	4.503	8.08E-03
132	4.504	1.05E-02
133	4.517	6.44E-04
134	4.521	6.58E-03
135	4.525	6.63E-03
136	4.531	1.62E-01
137	4.536	5.75E-02
138	4.542	7.86E-04
139	4.549	8.79E-02
140	4.557	9.23E-04
141	4.559	1.50E-03
142	4.570	9.76E-02
143	4.590	2.69E-02
144	4.613	9.57E-01
145	4.615	4.46E-05
146	4.651	3.68E-03
147	4.653	1.29E-02
148	4.656	2.00E-03
149	4.661	3.31E-04
150	4.687	2.48E-05
151	4.690	7.33E-05
152	4.697	4.23E-03
153	4.698	2.46E-03
154	4.704	1.43E-05
155	4.713	1.31E-02
156	4.713	5.05E-04
157	4.734	1.89E-03
158	4.746	8.93E-05
159	4.750	1.20E-03
160	4.762	1.93E-03

*Table S7: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Zn***

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
1	2.043	0.00E+00	3.17%	0.00%	5.20%	77.82%	0.02%	12.38%	0.03%	0.00%	0.29%	0.00%	1.09%
2	2.190	1.00E-03	2.75%	0.00%	4.49%	71.90%	0.02%	19.19%	0.04%	0.00%	0.28%	0.00%	1.32%
3	2.409	1.01E-01	1.39%	0.00%	11.66%	71.48%	0.02%	13.68%	0.06%	0.01%	0.49%	0.00%	1.22%
4	2.782	2.40E-02	2.66%	0.00%	5.29%	76.02%	0.03%	13.74%	0.04%	0.00%	0.88%	0.00%	1.34%
5	2.905	4.00E-03	1.99%	0.00%	13.15%	78.73%	0.02%	5.60%	0.02%	0.00%	0.02%	0.00%	0.47%
6	2.918	9.00E-03	2.40%	0.00%	5.10%	70.09%	0.02%	20.01%	0.03%	0.00%	0.79%	0.00%	1.58%
7	2.939	0.00E+00	4.83%	0.00%	11.86%	76.05%	0.02%	6.07%	0.02%	0.00%	0.02%	0.00%	1.13%
8	3.023	2.80E-02	1.19%	0.00%	9.65%	74.57%	0.01%	13.43%	0.03%	0.00%	0.39%	0.00%	0.72%
9	3.058	9.00E-02	2.02%	0.00%	20.34%	71.28%	0.02%	5.59%	0.03%	0.00%	0.01%	0.00%	0.72%
10	3.087	1.02E-01	0.80%	0.00%	9.38%	74.78%	0.02%	14.53%	0.04%	0.00%	0.11%	0.00%	0.33%
11	3.123	4.00E-02	4.04%	0.00%	13.41%	69.17%	0.02%	11.74%	0.04%	0.00%	0.11%	0.00%	1.47%
12	3.169	1.92E-01	4.10%	0.00%	14.61%	69.39%	0.01%	10.42%	0.03%	0.00%	0.01%	0.00%	1.42%
13	3.205	1.66E-01	1.09%	0.00%	9.25%	72.60%	0.02%	16.50%	0.03%	0.00%	0.09%	0.00%	0.43%
14	3.246	8.20E-02	0.84%	0.00%	12.16%	72.85%	0.01%	13.69%	0.01%	0.00%	0.09%	0.00%	0.36%
15	3.368	1.00E-03	0.02%	0.00%	1.60%	0.85%	0.00%	93.74%	0.01%	0.00%	0.00%	0.00%	3.78%
16	3.421	3.00E-03	0.02%	0.00%	1.56%	0.86%	0.00%	93.77%	0.01%	0.00%	0.01%	0.00%	3.78%
17	3.580	5.00E-02	1.97%	0.00%	16.20%	68.22%	0.02%	12.12%	0.07%	0.00%	0.10%	0.00%	1.31%
18	3.806	3.00E-03	4.15%	0.00%	15.88%	73.45%	0.02%	5.37%	0.03%	0.00%	0.06%	0.00%	1.05%
19	3.914	4.00E-03	43.17%	0.00%	6.00%	37.04%	0.01%	3.81%	0.02%	0.01%	0.22%	0.02%	9.71%
20	3.950	1.00E-03	48.02%	0.00%	5.12%	33.66%	0.00%	3.21%	0.01%	0.00%	0.11%	0.00%	9.86%
21	3.974	3.80E-02	7.27%	0.00%	20.26%	65.89%	0.02%	4.57%	0.03%	0.00%	0.06%	0.00%	1.88%
22	4.007	0.00E+00	0.00%	0.02%	0.08%	0.03%	2.69%	0.04%	93.63%	2.94%	0.00%	0.07%	0.50%
23	4.015	3.00E-03	1.39%	0.00%	25.07%	44.29%	0.02%	27.81%	0.09%	0.00%	0.03%	0.00%	1.30%
24	4.018	3.00E-03	5.26%	0.00%	14.69%	66.85%	0.02%	11.56%	0.19%	0.01%	0.05%	0.00%	1.39%
25	4.045	1.00E-03	0.55%	0.00%	6.81%	27.36%	0.01%	61.47%	0.09%	0.00%	0.01%	0.00%	3.71%
26	4.060	8.00E-03	48.83%	0.00%	4.68%	27.00%	0.05%	6.14%	0.70%	0.03%	0.13%	0.00%	12.45%
27	4.079	4.00E-03	1.37%	0.03%	7.83%	1.40%	4.15%	12.92%	68.54%	2.15%	0.01%	0.10%	1.51%
28	4.081	4.70E-02	1.02%	0.01%	9.92%	2.99%	0.83%	67.77%	13.72%	0.44%	0.01%	0.02%	3.29%
29	4.110	0.00E+00	0.00%	0.01%	0.30%	0.03%	1.93%	0.04%	94.24%	2.92%	0.00%	0.05%	0.48%
30	4.121	1.00E-02	2.71%	0.00%	15.41%	74.40%	0.02%	6.46%	0.16%	0.01%	0.02%	0.00%	0.82%
31	4.151	6.60E-02	0.71%	0.00%	16.09%	75.72%	0.02%	7.03%	0.08%	0.00%	0.01%	0.00%	0.34%
32	4.160	1.70E-02	0.52%	0.01%	25.85%	33.16%	1.47%	3.92%	32.82%	1.03%	0.02%	0.04%	1.16%
33	4.163	1.00E-02	0.33%	0.01%	21.63%	22.98%	2.06%	3.17%	47.23%	1.48%	0.01%	0.05%	1.06%
34	4.180	1.48E-01	0.88%	0.00%	35.56%	48.57%	0.01%	12.34%	0.21%	0.01%	0.02%	0.00%	2.39%
35	4.227	1.66E-01	0.93%	0.00%	55.63%	34.27%	0.01%	7.03%	0.03%	0.00%	0.02%	0.00%	2.09%
36	4.240	3.03E-01	1.13%	0.00%	38.80%	51.41%	0.02%	7.28%	0.03%	0.00%	0.02%	0.00%	1.32%
37	4.258	4.00E-03	3.89%	0.00%	16.70%	66.87%	0.01%	11.17%	0.04%	0.00%	0.01%	0.00%	1.31%
38	4.272	2.60E-02	0.24%	0.00%	82.21%	8.98%	0.00%	4.40%	0.01%	0.00%	0.00%	0.00%	4.16%
39	4.280	6.00E-03	1.18%	0.00%	61.32%	29.72%	0.01%	4.64%	0.02%	0.00%	0.01%	0.00%	3.10%
40	4.305	4.00E-03	0.04%	0.00%	3.64%	2.04%	0.00%	92.99%	0.00%	0.00%	0.00%	0.00%	1.28%
41	4.350	2.08E-01	0.60%	0.00%	19.55%	13.16%	0.01%	64.02%	0.02%	0.00%	0.00%	0.00%	2.64%
42	4.357	1.37E+00	1.22%	0.00%	47.09%	44.54%	0.01%	5.18%	0.02%	0.00%	0.01%	0.00%	1.94%
43	4.365	2.46E-01	0.73%	0.00%	40.83%	20.37%	0.01%	36.19%	0.03%	0.00%	0.00%	0.00%	1.85%
44	4.530	4.20E-02	6.79%	0.00%	13.85%	64.89%	0.07%	10.98%	0.36%	0.02%	0.15%	0.01%	2.90%
45	4.554	3.00E-03	46.73%	0.00%	5.41%	31.62%	0.01%	4.06%	0.04%	0.01%	0.21%	0.01%	11.91%
46	4.561	3.00E-03	46.44%	0.00%	5.48%	31.50%	0.01%	4.09%	0.03%	0.01%	0.22%	0.01%	12.21%
47	4.641	7.95E-01	0.05%	0.02%	77.83%	0.50%	0.10%	17.54%	0.12%	0.02%	0.00%	0.00%	3.82%
48	4.674	2.00E-03	41.81%	0.00%	7.24%	31.16%	0.04%	6.69%	0.26%	0.01%	0.14%	0.01%	12.64%
49	4.707	0.00E+00	0.00%	0.03%	0.06%	0.00%	2.64%	0.01%	92.02%	4.75%	0.00%	0.11%	0.39%
50	4.746	3.00E-03	0.09%	0.00%	2.60%	4.28%	0.20%	87.77%	1.41%	0.04%	0.01%	0.01%	3.59%
51	4.786	4.00E-03	0.02%	0.04%	6.06%	0.14%	4.57%	0.60%	83.63%	4.09%	0.00%	0.19%	0.68%
52	4.796	4.00E-03	1.79%	0.01%	6.38%	28.84%	1.70%	46.51%	11.82%	0.36%	0.06%	0.05%	2.49%
53	4.810	3.00E-03	0.01%	0.02%	0.65%	0.19%	1.87%	0.42%	91.85%	4.54%	0.00%	0.07%	0.38%
54	4.817	1.09E-01	0.05%	0.00%	10.08%	1.17%	0.10%	83.99%	0.98%	0.05%	0.01%	0.00%	3.58%
55	4.821	1.90E-02	0.78%	0.03%	6.62%	31.11%	5.90%	13.48%	39.52%	1.29%	0.07%	0.16%	1.04%
56	4.854	3.50E-02	1.05%	0.02%	4.42%	25.48%	3.60%	39.36%	23.43%	0.73%	0.03%	0.09%	1.80%
57	4.869	0.00E+00	0.01%	0.03%	8.95%	0.55%	3.41%	1.84%	80.31%	3.91%	0.01%	0.14%	0.84%
58	4.886	1.01E-01	0.89%	0.00%	20.04%	62.70%	0.06%	14.56%	0.49%	0.03%	0.07%	0.00%	1.16%
59	4.924	1.30E-02	1.44%	0.00%	8.37%	52.90%	0.67%	30.38%	4.24%	0.13%	0.07%	0.02%	1.79%
60	4.925	6.80E-02	0.25%	0.00%	10.93%	9.89%	0.10%	75.00%	0.51%	0.02%	0.03%	0.00%	3.28%
61	4.950	0.00E+00	0.00%	0.00%	0.07%	0.00%	2.63%	0.02%	95.77%	1.46%	0.00%	0.04%	0.01%
62	4.995	2.00E-03	0.08%	0.01%	8.30%	1.66%	0.85%	81.75%	3.79%	0.15%	0.01%	0.02%	3.39%
63	5.031	0.00E+00	0.00%	0.01%	6.04%	0.11%	4.68%	0.39%	87.19%	1.41%	0.00%	0.07%	0.12%
64	5.051	0.00E+00	0.00%	0.00%	1.20%	0.03%	1.96%	0.07%	95.25%	1.45%	0.00%	0.03%	0.02%
65	5.055	4.30E-02	0.05%	0.00%	93.08%	1.76%	0.06%	2.90%	1.25%	0.03%	0.01%	0.00%	0.86%
66	5.092	4.90E-02	0.03%	0.00%	92.83%	2.62%	0.04%	3.11%	0.29%	0.01%	0.00%	0.00%	1.08%
67	5.110	0.00E+00	0.01%	0.01%	11.34%	0.24%	3.72%	1.28%	81.88%	1.25%	0.00%	0.05%	0.23%
68	5.127	0.00E+00	0.00%	0.00%	0.16%	0.01%	2.66%	0.23%	94.45%	2.41%	0.00%	0.07%	0.02%
69	5.129	3.00E-03	0.05%	0.05%	23.26%	1.79%	8.95%	21.17%	41.32%	1.32%	0.01%	0.23%	1.85%
70	5.142	1.00E-03	0.22%	0.00%	8.39%	5.68%	0.73%	79.23%	2.39%	0.08%	0.03%	0.02%	3.24%
71	5.189	2.00E-03	0.17%	0.01%	72.32%	7.29%	0.24%	15.01%	0.82%	0.03%	0.10%	0.01%	4.01%
72	5.198	1.00E-03	0.00%	0.00%	2.21%	0.19%	2.89%	1.47%	88.92%	4.12%	0.00%	0.12%	0.06%
73	5.216	5.90E-02	0.06%	0.00%	76.95%	6.59%	0.45%	4.84%	9.66%	0.39%	0.00%	0.02%	1.04%
74	5.231	0.00E+00	0.00%	0.00%	0.80%	0.07%	1.94%	0.82%	93.89%	2.40%	0.00%	0.05%	0.03%
75	5.237	8.00E-03	0.01%	0.00%	7.60%	0.50%	3.93%	4.58%	80.64%	2.42%	0.00%	0.10%	0.20%
76	5.251	4.50E-02	0.03%	0.00%	91.47%	2.02%	0.10%	2.71%	1.40%	0.04%	0.00%	0.00%	2.23%
77	5.287	2.00E-03	0.17%	0.00%	38.12%	4.81%	1.56%	10.99%	41.35%	1.48%	0.09%	0.06%	1.39%
78	5.303	3.00E-03	0.12%	0.00%	15.20%	3.23%	1.77%	19.89%	55.80%	2.67%	0.04%	0.08%	1.20%
79	5.306	2.00E-03	0.05%	0.00%	2.71%	1.54%	3.82%	19.52%	67.80%	3.44%	0.01%	0.19%	0.93%
80	5.310	8.00E-03	0.20%	0.00%	28.75%	6.17%	1.27%	38.37%	21.83%	1.09%	0.05%	0.05%	2.23%

*Table S8: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Rh***

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
1	1.915	0.00E+00	3.61%	0.00%	4.86%	75.92%	0.03%	13.18%	0.86%	0.00%	0.00%	0.04%	1.50%
2	2.056	1.00E-03	3.21%	0.00%	4.43%	71.22%	0.02%	18.52%	0.85%	0.00%	0.00%	0.03%	1.74%
3	2.275	1.31E-01	1.75%	0.04%	11.49%	69.08%	0.44%	13.53%	1.36%	0.01%	0.06%	0.28%	1.97%
4	2.605	0.00E+00	0.00%	37.69%	0.28%	0.02%	5.27%	0.01%	0.06%	0.03%	18.10%	2.69%	35.85%
5	2.639	1.00E-03	0.01%	36.69%	0.35%	0.24%	5.15%	0.05%	1.01%	0.03%	17.49%	2.59%	36.40%
6	2.748	1.50E-02	2.41%	0.07%	3.83%	57.54%	0.06%	9.87%	13.18%	0.00%	0.03%	0.05%	12.97%
7	2.872	0.00E+00	1.55%	0.02%	2.24%	37.07%	0.02%	9.83%	23.68%	0.00%	0.01%	0.03%	25.54%

8	2.893	1.00E-02	1.33%	1.08%	2.98%	37.62%	0.36%	7.42%	22.47%	0.01%	0.55%	0.20%	25.98%
9	2.916	4.00E-03	0.09%	34.87%	0.93%	2.84%	11.01%	0.36%	1.14%	0.13%	17.47%	5.68%	25.50%
10	2.941	3.00E-03	2.43%	0.87%	11.64%	69.47%	0.31%	5.08%	4.48%	0.01%	0.55%	0.23%	4.95%
11	2.947	8.00E-03	1.95%	0.49%	5.74%	46.64%	0.33%	7.61%	16.11%	0.01%	0.32%	0.28%	20.52%
12	2.975	3.50E-02	2.97%	0.37%	7.91%	52.91%	0.31%	5.74%	12.52%	0.01%	0.28%	0.32%	16.66%
13	3.016	1.00E-03	0.79%	0.21%	2.01%	26.54%	0.16%	6.57%	27.71%	0.00%	0.12%	0.15%	35.74%
14	3.021	1.10E-02	1.59%	0.28%	6.89%	64.66%	0.16%	9.59%	6.95%	0.05%	0.24%	0.17%	9.49%
15	3.042	2.00E-03	0.02%	23.42%	1.08%	0.84%	14.06%	0.25%	0.43%	0.27%	18.03%	13.92%	27.70%
16	3.065	1.80E-02	2.53%	0.18%	3.78%	28.79%	0.95%	4.13%	31.77%	0.03%	0.18%	0.96%	26.71%
17	3.069	6.10E-02	0.83%	0.95%	6.18%	34.91%	16.34%	7.20%	6.51%	0.46%	0.63%	16.94%	9.06%
18	3.072	2.50E-02	0.72%	0.92%	4.83%	21.24%	25.68%	4.35%	6.06%	0.75%	0.68%	27.16%	7.63%
19	3.084	7.50E-02	2.31%	0.03%	17.04%	65.30%	0.54%	5.04%	4.39%	0.02%	0.03%	0.58%	4.73%
20	3.123	4.70E-02	1.92%	0.52%	8.38%	62.84%	0.65%	12.87%	5.44%	0.02%	0.36%	0.64%	6.38%
21	3.142	3.90E-02	0.09%	5.16%	3.24%	3.32%	31.31%	5.04%	0.50%	1.13%	3.85%	39.73%	6.63%
22	3.162	1.30E-01	2.03%	1.39%	8.04%	48.55%	1.51%	11.55%	11.28%	0.04%	0.93%	1.53%	13.16%
23	3.172	1.54E-01	2.75%	0.12%	10.61%	60.65%	0.15%	11.37%	6.74%	0.00%	0.10%	0.15%	7.36%
24	3.181	1.50E-02	2.12%	2.99%	8.05%	37.52%	1.43%	5.03%	18.31%	0.03%	2.01%	1.19%	21.32%
25	3.190	2.10E-02	0.42%	3.13%	2.46%	6.39%	6.02%	58.11%	3.67%	0.19%	2.49%	6.41%	10.73%
26	3.191	6.50E-02	2.27%	0.60%	5.15%	27.08%	0.89%	14.88%	23.60%	0.03%	0.42%	0.90%	24.17%
27	3.214	2.00E-03	0.12%	5.73%	2.27%	2.69%	24.42%	18.53%	0.07%	0.96%	4.78%	31.07%	9.37%
28	3.216	5.80E-02	2.09%	0.18%	13.17%	69.20%	0.70%	11.76%	0.51%	0.03%	0.14%	0.85%	1.37%
29	3.245	4.00E-03	0.03%	0.16%	1.53%	1.02%	0.70%	90.16%	0.02%	0.03%	0.13%	0.82%	5.41%
30	3.254	0.00E+00	0.01%	25.65%	1.09%	0.17%	14.69%	0.47%	0.33%	0.43%	19.30%	14.21%	23.66%
31	3.312	3.00E-03	0.39%	26.51%	0.82%	2.59%	8.29%	0.56%	6.30%	0.16%	19.46%	6.09%	28.86%
32	3.571	3.20E-02	2.31%	0.00%	16.67%	68.51%	0.07%	10.19%	0.36%	0.01%	0.01%	0.08%	1.80%
33	3.614	0.00E+00	0.00%	0.05%	1.46%	0.01%	0.53%	0.03%	0.00%	2.18%	9.58%	80.78%	5.40%
34	3.691	0.00E+00	0.00%	0.10%	3.30%	0.03%	0.80%	0.11%	0.00%	2.11%	9.09%	78.88%	5.58%
35	3.723	2.30E-02	0.01%	0.19%	1.69%	0.15%	3.01%	0.18%	0.01%	2.18%	7.86%	80.20%	4.54%
36	3.751	2.00E-03	0.00%	0.30%	0.33%	0.01%	0.18%	0.01%	0.00%	0.57%	48.02%	18.21%	32.38%
37	3.847	8.00E-03	0.01%	0.55%	0.90%	0.38%	0.36%	0.10%	0.01%	0.60%	45.99%	17.92%	33.20%
38	3.850	1.00E-03	2.94%	0.01%	17.33%	72.52%	0.08%	5.08%	0.28%	0.01%	0.26%	0.18%	1.32%
39	3.865	9.00E-03	0.00%	1.31%	0.48%	0.03%	1.46%	0.33%	0.06%	0.47%	46.35%	15.76%	33.75%
40	3.874	0.00E+00	0.02%	0.04%	1.03%	0.33%	0.05%	20.62%	0.29%	0.01%	0.43%	0.19%	77.01%
41	3.926	2.00E-03	0.06%	0.15%	1.47%	0.91%	7.87%	18.90%	0.43%	0.44%	0.64%	9.57%	59.56%
42	3.932	1.70E-02	0.07%	0.56%	2.84%	0.25%	32.45%	3.34%	0.12%	1.82%	0.71%	39.72%	18.13%
43	3.954	1.00E-03	45.46%	0.00%	4.31%	32.02%	0.13%	3.43%	2.38%	0.02%	0.04%	0.16%	12.05%
44	3.974	0.00E+00	49.15%	0.00%	4.79%	31.70%	0.14%	2.91%	0.59%	0.01%	0.04%	0.19%	10.49%
45	3.979	9.00E-03	0.19%	0.46%	2.43%	0.25%	22.71%	3.63%	0.01%	1.36%	21.79%	34.06%	13.14%
46	3.991	0.00E+00	0.11%	0.47%	2.04%	0.29%	13.56%	4.38%	0.01%	0.96%	33.44%	26.34%	18.40%
47	4.010	4.10E-02	3.26%	0.01%	20.79%	67.33%	0.49%	5.79%	0.10%	0.03%	0.02%	0.61%	1.59%
48	4.014	5.00E-03	0.43%	0.27%	10.12%	6.20%	13.79%	37.93%	0.06%	0.81%	0.35%	17.90%	12.15%
49	4.028	0.12%	0.12%	0.59%	6.73%	3.55%	27.55%	13.36%	0.04%	1.63%	2.11%	38.35%	5.99%
50	4.054	9.00E-03	1.39%	0.01%	22.24%	48.83%	0.50%	20.11%	0.09%	0.02%	0.02%	0.61%	6.18%
51	4.060	1.80E-02	2.29%	0.01%	9.90%	36.11%	0.41%	39.66%	0.09%	0.01%	0.01%	0.46%	11.05%
52	4.064	1.60E-02	2.32%	0.00%	11.93%	37.34%	0.18%	37.53%	0.09%	0.01%	0.03%	0.24%	10.34%
53	4.098	5.90E-02	13.35%	0.40%	2.18%	7.58%	6.09%	1.24%	0.29%	0.40%	32.00%	17.04%	19.45%
54	4.099	2.30E-02	36.06%	0.14%	3.19%	19.79%	2.26%	3.10%	0.91%	0.17%	11.96%	6.37%	16.05%
55	4.107	2.00E-03	0.17%	0.70%	0.70%	0.21%	1.22%	0.39%	0.07%	0.51%	52.25%	18.34%	25.43%
56	4.123	1.50E-02	0.01%	0.47%	2.70%	0.26%	34.05%	0.46%	0.01%	0.79%	10.11%	45.23%	5.93%
57	4.134	1.40E-02	0.07%	0.24%	4.18%	1.52%	30.90%	6.75%	0.03%	0.60%	2.35%	38.92%	14.44%
58	4.136	1.10E-02	0.29%	0.07%	6.08%	6.02%	8.19%	13.08%	0.22%	0.15%	0.19%	10.00%	55.72%
59	4.157	4.00E-03	0.02%	0.28%	4.10%	0.49%	39.49%	2.58%	0.00%	0.84%	0.53%	50.41%	1.26%
60	4.163	3.00E-03	2.10%	0.00%	15.56%	75.27%	0.04%	5.87%	0.06%	0.00%	0.13%	0.10%	0.87%
61	4.169	2.38E-01	0.70%	0.01%	35.17%	19.56%	1.40%	13.27%	0.31%	0.03%	0.14%	1.99%	27.41%
62	4.187	6.20E-02	0.79%	0.00%	30.21%	51.97%	0.16%	10.04%	0.05%	0.00%	0.03%	0.24%	6.52%
63	4.194	2.40E-02	0.20%	0.01%	8.59%	22.15%	0.75%	37.17%	0.27%	0.02%	0.14%	1.05%	29.66%
64	4.197	7.50E-02	0.48%	0.01%	16.74%	50.98%	0.61%	25.59%	0.04%	0.01%	0.03%	0.75%	4.78%
65	4.206	6.20E-02	0.29%	0.01%	17.82%	21.54%	0.46%	40.28%	0.17%	0.01%	0.05%	0.60%	18.78%
66	4.243	2.00E-03	0.03%	0.00%	7.04%	1.53%	0.26%	87.16%	0.01%	0.01%	0.01%	0.32%	3.63%
67	4.254	1.38E-01	0.56%	0.00%	48.89%	36.88%	0.10%	9.00%	0.08%	0.00%	0.00%	0.13%	4.36%
68	4.266	2.52E-01	1.06%	0.00%	38.40%	47.24%	0.06%	7.61%	0.10%	0.00%	0.01%	0.06%	5.47%
69	4.277	1.05E-01	0.28%	0.00%	76.76%	13.23%	0.08%	4.00%	0.03%	0.00%	0.00%	0.09%	5.53%
70	4.295	4.30E-02	1.06%	0.00%	63.71%	25.81%	0.05%	6.11%	0.03%	0.00%	0.00%	0.07%	3.17%
71	4.300	6.00E-03	5.13%	0.00%	15.81%	66.43%	0.11%	10.60%	0.08%	0.00%	0.00%	0.10%	1.75%
72	4.386	3.50E-02	2.26%	0.00%	40.54%	48.77%	0.07%	6.23%	0.03%	0.00%	0.00%	0.09%	2.00%
73	4.391	1.18E+00	0.95%	0.00%	38.75%	53.89%	0.10%	4.62%	0.02%	0.01%	0.00%	0.12%	1.54%
74	4.449	0.00E+00	0.02%	0.02%	3.03%	0.03%	1.33%	0.46%	0.00%	3.68%	1.60%	88.98%	0.84%
75	4.474	2.00E-03	0.00%	0.03%	0.17%	0.05%	41.62%	3.70%	0.00%	1.31%	0.01%	51.96%	1.14%
76	4.512	5.03E-01	0.06%	0.38%	57.52%	0.51%	1.21%	19.52%	0.02%	0.20%	1.74%	9.15%	9.69%
77	4.520	1.30E-02	1.91%	0.02%	4.29%	18.24%	29.11%	6.25%	0.08%	1.10%	0.05%	37.26%	1.69%
78	4.529	2.10E-02	3.87%	0.03%	8.10%	33.02%	11.54%	7.98%	0.16%	0.94%	0.39%	31.59%	2.38%
79	4.533	1.40E-02	1.16%	0.04%	5.51%	8.59%	3.84%	2.75%	0.04%	2.84%	1.37%	72.28%	1.56%
80	4.540	1.00E-03	0.06%	0.01%	0.27%	0.30%	40.11%	3.88%	0.00%	2.46%	0.04%	50.68%	2.20%

*Table S9: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Pd***

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
1	1.962	0.00E+00	3.35%	0.00%	5.08%	76.97%	0.05%	12.12%	0.01%	0.00%	1.10%	0.00%	1.32%
2	2.115	1.00E-03	2.90%	0.00%	4.29%	70.79%	0.05%	19.20%	0.01%	0.00%	1.08%	0.00%	1.67%
3	2.306	1.32E-01	1.61%	0.02%	11.39%	69.77%	0.44%	13.24%	0.28%	0.05%	1.53%	0.01%	1.67%
4	2.596	1.00E-03	1.71%	2.61%	1.36%	15.22%	0.96%	2.55%	0.08%	0.16%	38.18%	0.02%	37.15%
5	2.666	2.00E-03	0.08%	35.03%	0.86%	0.85%	12.59%	0.18%	4.97%	13.53%	1.93%	0.22%	29.76%
6	2.670	4.00E-03	0.16%	37.62%	1.02%	1.72%	13.68%	0.33%	3.22%	8.17%	3.81%	0.24%	30.06%
7	2.704	1.00E-03	0.94%	6.44%	2.45%	11.47%	2.21%	2.17%	1.01%	2.88%	30.37%	0.04%	40.03%
8	2.742	1.00E-03	1.60%	4.13%	1.02%	12.98%	1.53%	3.82%	0.31%	0.69%	33.65%	0.03%	40.25%
9	2.782	7.00E-03	1.50%	14.56%	3.07%	39.94%	5.02%	6.55%	3.45%	9.87%	1.38%	0.08%	14.60%
10	2.793	1.40E-02	1.36%	16.80%	2.78%	35.51%	5.93%	6.04%	3.72%	10.55%	1.14%	0.10%	16.07%
11	2.885	1.00E-03	0.27%	28.73%	1.15%	2.98%	9.88%	0.62%	4.29%	12.32%	7.36%	0.17%	32.23%
12	2.915	1.92%	1.92%	0.00%	12.54%	78.64%	0.03%	5.10%	0.01%	0.00%	0.72%	0.00%	1.05%
13	2.924	9.00E-03	2.59%	0.06%	4.86%	70.17%	0.13%	18.20%	0.04%	0.02%	2.14%	0.00%	1.78%
14	2.937	1.00E-03	5.11%	0.00%	11.28%	76.87%	0.03%	5.55%	0.01%	0.00%	0.06%	0.00%	1.09%
15	3.025	2.40E-02	1.27%	0.00%	9.21%	74.11%	0.12%	13.13%	0.08%	0.00%	1.15%	0.01%	0.93%

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
16	3.063	9.50E-02	2.08%	0.00%	19.21%	72.28%	0.04%	5.09%	0.02%	0.00%	0.30%	0.00%	0.98%
17	3.071	1.83E-01	1.19%	0.02%	9.09%	74.28%	0.14%	13.42%	0.09%	0.03%	0.83%	0.00%	0.91%
18	3.129	9.00E-03	3.61%	0.00%	14.20%	70.00%	0.13%	10.40%	0.07%	0.01%	0.24%	0.01%	1.33%
19	3.155	1.60E-02	0.27%	2.11%	4.56%	4.59%	43.45%	0.75%	39.99%	1.94%	0.01%	1.02%	1.32%
20	3.165	1.87E-01	3.99%	0.16%	13.37%	65.40%	3.01%	9.52%	2.83%	0.14%	0.09%	0.06%	1.44%
21	3.181	1.51E-01	1.05%	0.00%	8.20%	73.48%	0.08%	16.18%	0.05%	0.03%	0.36%	0.00%	0.57%
22	3.184	3.00E-03	0.00%	2.03%	4.92%	0.11%	80.93%	0.18%	8.75%	0.47%	0.00%	1.81%	0.79%
23	3.237	6.00E-02	0.79%	0.03%	11.92%	72.34%	0.21%	13.56%	0.18%	0.01%	0.41%	0.00%	0.56%
24	3.274	4.00E-03	0.01%	0.02%	1.53%	0.52%	0.54%	91.89%	0.39%	0.03%	0.01%	0.02%	5.05%
25	3.328	3.00E-03	0.02%	0.00%	1.45%	0.91%	0.03%	92.44%	0.04%	0.00%	0.02%	0.00%	5.07%
26	3.424	6.20E-02	0.07%	1.15%	5.56%	1.16%	46.58%	1.35%	39.86%	1.98%	0.01%	1.29%	1.00%
27	3.453	0.00E+00	0.00%	0.92%	3.46%	0.02%	32.52%	0.07%	58.59%	2.98%	0.00%	0.70%	0.75%
28	3.553	4.90E-02	2.20%	0.01%	15.72%	66.92%	0.07%	9.59%	0.73%	1.96%	0.21%	0.00%	2.58%
29	3.561	1.00E-02	0.10%	0.30%	1.27%	2.70%	0.16%	0.48%	17.06%	49.15%	0.02%	0.00%	28.78%
30	3.710	0.00E+00	0.00%	0.02%	3.71%	0.02%	0.69%	0.14%	90.27%	4.35%	0.00%	0.02%	0.80%
31	3.716	0.00E+00	0.03%	0.01%	0.64%	0.13%	0.00%	18.37%	0.16%	0.02%	0.27%	0.00%	80.37%
32	3.770	2.00E-03	0.35%	0.00%	0.72%	0.43%	0.00%	18.22%	0.00%	0.01%	0.42%	0.00%	79.85%
33	3.813	3.00E-03	3.41%	0.00%	16.21%	74.18%	0.05%	4.97%	0.03%	0.00%	0.16%	0.00%	0.98%
34	3.929	4.00E-03	43.37%	0.00%	5.42%	36.05%	0.10%	3.56%	0.07%	0.01%	1.09%	0.02%	10.30%
35	3.957	2.40E-02	0.04%	1.28%	4.66%	1.37%	41.99%	0.61%	44.65%	3.11%	0.00%	1.80%	0.50%
36	3.958	0.00E+00	50.39%	0.00%	4.49%	31.50%	0.04%	2.88%	0.04%	0.01%	0.26%	0.01%	10.41%
37	3.979	4.40E-02	7.24%	0.02%	19.65%	65.40%	0.65%	4.25%	0.66%	0.04%	0.20%	0.03%	1.86%
38	4.011	4.00E-03	0.75%	0.00%	27.07%	32.54%	0.17%	37.10%	0.11%	0.01%	0.05%	0.01%	2.19%
39	4.026	5.00E-03	4.13%	0.00%	13.37%	72.25%	0.11%	8.95%	0.09%	0.00%	0.09%	0.00%	1.00%
40	4.037	4.00E-03	0.05%	1.77%	3.90%	0.12%	79.14%	0.25%	10.03%	0.72%	0.00%	3.60%	0.44%
41	4.047	1.00E-03	0.66%	0.01%	8.69%	32.71%	0.29%	53.02%	0.22%	0.01%	0.02%	0.01%	4.37%
42	4.074	4.00E-02	26.97%	0.00%	8.28%	16.26%	0.07%	38.60%	0.07%	0.01%	0.28%	0.01%	9.45%
43	4.083	1.80E-02	23.55%	0.00%	6.21%	14.28%	0.15%	46.33%	0.20%	0.02%	0.24%	0.01%	8.99%
44	4.126	1.20E-02	2.45%	0.00%	14.51%	76.17%	0.13%	5.85%	0.12%	0.01%	0.05%	0.01%	0.71%
45	4.135	1.00E-03	0.02%	0.76%	4.78%	0.35%	44.57%	0.71%	45.19%	1.91%	0.01%	1.33%	0.40%
46	4.160	3.50E-02	0.82%	0.00%	36.93%	55.49%	0.05%	5.25%	0.02%	0.00%	0.05%	0.00%	1.40%
47	4.162	8.10E-02	0.64%	0.00%	16.79%	75.64%	0.05%	6.49%	0.03%	0.00%	0.03%	0.00%	0.33%
48	4.172	1.87E-01	0.91%	0.00%	40.86%	43.45%	0.06%	11.81%	0.05%	0.00%	0.04%	0.00%	2.83%
49	4.228	3.60E-02	0.24%	0.40%	17.47%	9.49%	62.00%	1.72%	6.98%	0.16%	0.01%	0.82%	0.71%
50	4.229	1.21E-01	0.68%	0.14%	40.27%	27.95%	21.57%	4.92%	2.51%	0.05%	0.03%	0.29%	1.60%
51	4.234	1.00E-03	0.00%	1.67%	3.91%	0.05%	32.06%	0.14%	52.06%	5.80%	0.00%	1.42%	2.89%
52	4.240	3.20E-01	1.01%	0.00%	33.39%	55.43%	0.09%	8.87%	0.08%	0.00%	0.05%	0.00%	1.09%
53	4.262	7.00E-03	3.16%	0.00%	34.05%	41.83%	0.08%	18.08%	0.08%	0.00%	0.02%	0.00%	2.70%
54	4.268	8.00E-03	1.40%	0.00%	34.54%	27.92%	0.24%	32.60%	0.17%	0.00%	0.01%	0.01%	3.11%
55	4.278	2.60E-02	0.09%	0.00%	37.93%	5.15%	0.35%	54.42%	0.25%	0.00%	0.00%	0.00%	1.80%
56	4.280	1.17E-01	0.28%	0.94%	13.43%	4.95%	37.53%	2.06%	37.02%	1.71%	0.00%	0.98%	1.09%
57	4.282	5.00E-03	0.85%	0.16%	55.47%	21.48%	6.37%	5.60%	6.41%	0.31%	0.01%	0.18%	3.17%
58	4.318	0.00E+00	0.01%	11.74%	4.29%	0.04%	6.17%	0.12%	13.44%	26.74%	0.05%	0.15%	37.27%
59	4.326	1.30E-02	0.17%	0.03%	2.13%	3.53%	1.16%	89.45%	1.40%	0.06%	0.01%	0.03%	2.04%
60	4.367	1.28E+00	1.02%	0.01%	43.02%	47.71%	1.17%	4.33%	1.04%	0.02%	0.02%	0.01%	1.66%
61	4.369	3.62E-01	1.49%	0.00%	50.30%	37.94%	0.11%	7.75%	0.08%	0.00%	0.02%	0.00%	2.31%
62	4.370	3.00E-02	0.03%	0.38%	11.51%	1.50%	46.30%	1.75%	36.49%	0.76%	0.01%	0.62%	0.65%
63	4.398	0.00E+00	0.00%	0.16%	4.24%	0.03%	20.74%	0.12%	70.71%	3.37%	0.00%	0.28%	0.35%
64	4.459	2.00E-03	0.00%	0.01%	0.26%	0.03%	39.69%	4.29%	53.19%	1.34%	0.00%	0.99%	0.20%
65	4.510	5.82E-01	0.04%	0.29%	57.42%	0.35%	9.28%	6.08%	19.74%	1.43%	0.01%	0.27%	5.09%
66	4.525	4.10E-02	6.69%	0.01%	14.06%	63.62%	0.73%	10.44%	1.07%	0.13%	0.29%	0.04%	2.93%
67	4.531	0.00E+00	0.10%	0.00%	0.23%	0.74%	38.61%	4.23%	51.28%	2.60%	0.00%	1.95%	0.26%
68	4.546	0.00E+00	0.04%	0.76%	3.61%	0.10%	16.69%	0.14%	71.39%	5.47%	0.00%	0.23%	1.58%
69	4.566	4.00E-03	46.38%	0.00%	5.89%	31.63%	0.11%	3.57%	0.12%	0.03%	0.21%	0.03%	12.03%
70	4.572	2.00E-03	46.39%	0.05%	5.16%	31.21%	0.12%	4.41%	0.07%	0.06%	0.28%	0.01%	12.26%
71	4.606	0.00E+00	0.03%	0.03%	0.10%	0.06%	79.87%	3.69%	13.83%	0.35%	0.00%	1.92%	0.13%
72	4.607	0.00E+00	0.03%	16.25%	0.76%	0.04%	6.93%	0.11%	15.16%	32.95%	0.01%	0.11%	27.66%
73	4.657	1.00E-03	0.28%	0.01%	2.81%	0.96%	0.05%	90.52%	0.31%	0.03%	0.01%	0.00%	5.01%
74	4.663	1.00E-03	4.80%	0.11%	1.09%	3.81%	40.54%	6.39%	38.86%	1.27%	0.04%	1.06%	2.03%
75	4.669	0.00E+00	0.24%	5.83%	14.05%	0.36%	2.23%	1.12%	2.33%	4.32%	0.53%	0.03%	68.96%
76	4.678	0.00E+00	0.90%	0.00%	0.23%	0.74%	76.13%	3.96%	13.06%	0.66%	0.01%	3.85%	0.46%
77	4.681	2.00E-03	30.63%	0.01%	6.19%	23.57%	6.83%	16.46%	5.62%	0.17%	0.22%	0.23%	10.08%
78	4.693	5.00E-03	0.05%	0.16%	5.86%	1.35%	5.31%	74.97%	7.16%	0.44%	0.02%	0.12%	4.55%
79	4.713	0.00E+00	0.00%	0.06%	3.82%	0.04%	1.92%	0.18%	91.47%	1.84%	0.00%	0.03%	0.64%
80	4.737	1.00E-03	0.04%	0.00%	0.33%	0.28%	44.44%	5.88%	44.23%	2.24%	0.00%	2.24%	0.32%

*Table S10: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Cd***

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
1	2.096	0.00E+00	3.34%	0.00%	5.30%	77.89%	0.03%	12.15%	0.03%	0.00%	0.29%	0.00%	0.97%
2	2.239	1.00E-03	2.91%	0.00%	4.63%	71.99%	0.03%	18.91%	0.03%	0.00%	0.29%	0.00%	1.22%
3	2.432	1.22E-01	1.66%	0.00%	11.89%	71.32%	0.01%	13.53%	0.04%	0.01%	0.44%	0.00%	1.09%
4	2.843	2.40E-02	2.38%	0.00%	5.48%	76.88%	0.03%	13.31%	0.03%	0.00%	0.87%	0.00%	1.02%
5	2.883	3.00E-03	2.18%	0.00%	12.98%	78.71%	0.03%	5.58%	0.02%	0.00%	0.01%	0.00%	0.49%
6	2.909	1.00E-03	5.00%	0.00%	11.85%	76.27%	0.02%	5.73%	0.02%	0.00%	0.01%	0.00%	1.10%
7	2.974	1.10E-02	2.24%	0.00%	5.45%	70.62%	0.02%	19.58%	0.03%	0.00%	0.77%	0.00%	1.29%
8	3.025	9.70E-02	2.04%	0.00%	20.18%	71.46%	0.02%	5.56%	0.03%	0.00%	0.01%	0.00%	0.70%
9	3.046	5.80E-02	0.45%	0.00%	12.80%	72.91%	0.01%	13.09%	0.02%	0.00%	0.33%	0.00%	0.39%
10	3.087	0.00E+00	2.70%	0.00%	10.06%	74.82%	0.02%	11.35%	0.02%	0.00%	0.13%	0.00%	0.90%
11	3.105	1.57E-01	3.42%	0.00%	11.97%	72.93%	0.03%	10.35%	0.03%	0.00%	0.14%	0.00%	1.13%
12	3.122	1.87E-01	4.36%	0.00%	14.07%	69.77%	0.01%	10.33%	0.02%	0.00%	0.02%	0.00%	1.43%
13	3.221	8.10E-02	0.89%	0.00%	7.04%	73.95%	0.03%	17.70%	0.02%	0.00%	0.05%	0.00%	0.32%
14	3.291	9.40E-02	0.87%	0.00%	12.30%	72.62%	0.01%	13.77%	0.01%	0.00%	0.06%	0.00%	0.37%
15	3.447	0.00E+00	0.04%	0.00%	1.99%	1.95%	0.00%	92.28%	0.00%	0.00%	0.01%	0.00%	3.73%
16	3.501	4.00E-03	0.03%	0.00%	1.81%	0.82%	0.00%	93.59%	0.01%	0.00%	0.01%	0.00%	3.75%
17	3.541	5.50E-02	2.09%	0.00%	15.12%	69.09%	0.02%	12.23%	0.02%	0.00%	0.09%	0.00%	1.34%
18	3.787	4.00E-03	2.21%	0.00%	16.05%	75.41%	0.03%	5.58%	0.03%	0.00%	0.06%	0.00%	0.63%
19	3.910	1.10E-02	35.13%	0.00%	8.77%	44.76%	0.01%	3.85%	0.01%	0.01%	0.21%	0.02%	7.24%
20	3.941	3.40E-02	18.27%	0.00%	15.77%	57.68%	0.02%	4.19%	0.02%	0.01%	0.12%	0.01%	3.92%
21	3.948	1.00E-03	39.40%	0.00%	6.36%	41.31%	0.00%	4.42%	0.01%	0.00%	0.45%	0.00%	8.05%
22	3.987	0.00E+00	2.45%	0.00%	24.78%	66.13%	0.03%	5.63%	0.02%	0.00%	0.03%	0.00%	0.93%
23	3.993	5.00E-03	14.15%	0.00%	13.36%	60.87%	0.01%	8.24%	0.02%	0.00%	0.13%	0.00%	3.22%

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
24	4.071	6.00E-03	50.97%	0.00%	4.19%	27.32%	0.00%	3.74%	0.02%	0.01%	0.42%	0.01%	13.33%
25	4.083	3.00E-03	2.41%	0.00%	14.28%	74.24%	0.02%	8.26%	0.02%	0.00%	0.02%	0.00%	0.76%
26	4.104	2.70E-02	0.44%	0.00%	24.18%	23.65%	0.00%	50.09%	0.01%	0.00%	0.02%	0.00%	1.62%
27	4.112	6.40E-02	0.70%	0.00%	18.83%	71.24%	0.02%	8.78%	0.04%	0.00%	0.01%	0.00%	0.36%
28	4.134	1.55E-01	0.89%	0.00%	31.09%	42.11%	0.01%	24.70%	0.06%	0.00%	0.03%	0.00%	1.10%
29	4.136	1.00E-03	0.73%	0.00%	16.54%	49.30%	0.01%	31.23%	0.02%	0.00%	0.03%	0.00%	2.14%
30	4.145	4.00E-03	0.02%	0.03%	9.50%	0.22%	4.72%	0.52%	81.56%	2.71%	0.00%	0.13%	0.59%
31	4.174	0.00E+00	0.00%	0.02%	0.05%	0.01%	2.81%	0.01%	93.68%	3.09%	0.00%	0.08%	0.26%
32	4.177	5.90E-02	0.39%	0.00%	10.95%	31.05%	0.01%	54.93%	0.03%	0.00%	0.04%	0.00%	2.62%
33	4.211	1.78E-01	1.72%	0.00%	29.15%	49.26%	0.02%	17.38%	0.04%	0.00%	0.05%	0.00%	2.40%
34	4.213	1.27E-01	0.87%	0.00%	43.10%	37.62%	0.01%	15.54%	0.04%	0.00%	0.03%	0.00%	2.79%
35	4.217	0.00E+00	0.01%	0.02%	0.17%	0.19%	2.22%	0.05%	93.84%	3.15%	0.00%	0.06%	0.30%
36	4.219	7.00E-03	3.42%	0.00%	16.62%	67.00%	0.01%	11.44%	0.28%	0.01%	0.01%	0.00%	1.20%
37	4.251	2.00E-03	0.03%	0.02%	20.32%	0.64%	2.98%	1.70%	70.88%	2.36%	0.00%	0.08%	1.00%
38	4.269	3.40E-02	1.00%	0.00%	64.51%	26.90%	0.02%	4.32%	0.35%	0.01%	0.01%	0.00%	2.88%
39	4.278	9.00E-03	0.03%	0.00%	90.33%	1.52%	0.00%	3.74%	0.00%	0.00%	0.00%	0.00%	4.38%
40	4.342	1.48E+00	0.84%	0.00%	51.39%	37.59%	0.01%	7.71%	0.01%	0.00%	0.01%	0.00%	2.44%
41	4.349	4.14E-01	0.91%	0.00%	66.33%	24.46%	0.01%	4.54%	0.03%	0.00%	0.03%	0.00%	3.69%
42	4.384	6.30E-02	0.01%	0.00%	3.69%	1.17%	0.00%	93.75%	0.00%	0.00%	0.00%	0.00%	1.37%
43	4.433	1.00E-03	0.16%	0.00%	2.34%	1.81%	0.00%	94.24%	0.01%	0.00%	0.07%	0.00%	1.38%
44	4.465	1.70E-02	5.37%	0.02%	4.11%	23.85%	0.01%	4.00%	0.04%	0.03%	35.33%	0.00%	27.24%
45	4.508	1.80E-02	6.13%	0.00%	9.74%	47.53%	0.03%	8.21%	0.18%	0.01%	14.92%	0.00%	13.25%
46	4.531	1.00E-03	31.94%	0.00%	4.02%	24.71%	0.01%	3.62%	0.03%	0.01%	14.74%	0.00%	20.93%
47	4.563	0.00E+00	33.66%	0.00%	5.01%	28.13%	0.01%	4.19%	0.05%	0.01%	11.13%	0.01%	17.80%
48	4.624	0.00E+00	11.81%	0.01%	3.76%	23.24%	0.02%	4.54%	0.10%	0.02%	28.30%	0.00%	28.20%
49	4.644	7.00E-03	16.15%	0.01%	3.47%	17.99%	0.01%	3.14%	0.06%	0.01%	29.21%	0.00%	29.96%
50	4.675	8.63E-01	0.12%	0.02%	82.13%	0.56%	0.07%	12.65%	0.14%	0.04%	0.17%	0.00%	4.09%
51	4.686	2.00E-03	38.98%	0.00%	7.14%	28.97%	0.09%	5.94%	0.51%	0.03%	3.65%	0.01%	14.68%
52	4.751	0.00E+00	1.18%	0.03%	41.40%	3.27%	4.39%	26.97%	18.91%	0.57%	0.04%	0.13%	3.13%
53	4.809	1.00E-03	1.45%	0.00%	5.15%	44.13%	0.41%	43.06%	3.07%	0.10%	0.33%	0.01%	2.28%
54	4.833	1.20E-02	0.65%	0.03%	6.13%	20.32%	4.93%	26.87%	37.97%	1.30%	0.16%	0.13%	1.51%
55	4.844	5.00E-03	0.02%	0.04%	9.83%	0.19%	4.57%	0.80%	80.19%	3.52%	0.00%	0.18%	0.67%
56	4.866	1.20E-02	0.31%	0.03%	7.48%	8.97%	5.32%	35.80%	38.93%	1.34%	0.02%	0.15%	1.66%
57	4.873	0.00E+00	0.00%	0.02%	0.06%	0.01%	2.76%	0.03%	92.75%	4.09%	0.00%	0.10%	0.19%
58	4.885	1.34E-01	0.14%	0.01%	12.72%	7.32%	0.37%	74.03%	1.91%	0.08%	0.02%	0.01%	3.39%
59	4.899	2.10E-02	0.86%	0.00%	16.83%	58.36%	0.12%	21.29%	1.20%	0.05%	0.14%	0.00%	1.14%
60	4.911	2.50E-02	1.64%	0.00%	11.57%	52.55%	0.54%	29.56%	2.09%	0.08%	0.20%	0.02%	1.75%
61	4.915	0.00E+00	0.01%	0.02%	0.27%	0.80%	2.16%	0.29%	91.96%	4.19%	0.00%	0.08%	0.22%
62	4.937	0.00E+00	0.02%	0.03%	21.08%	0.75%	3.35%	3.20%	67.27%	3.01%	0.01%	0.11%	1.19%
63	4.952	7.00E-03	0.06%	0.06%	27.95%	1.06%	8.45%	19.24%	39.63%	1.39%	0.02%	0.23%	1.93%
64	4.968	1.00E-03	0.61%	0.01%	10.49%	17.87%	0.74%	63.37%	3.56%	0.15%	0.07%	0.02%	3.11%
65	4.996	4.60E-02	0.13%	0.01%	13.18%	4.18%	1.50%	70.69%	6.68%	0.23%	0.02%	0.04%	3.34%
66	5.035	3.80E-02	0.02%	0.00%	93.89%	1.62%	0.01%	3.41%	0.03%	0.00%	0.00%	0.00%	1.03%
67	5.090	0.00E+00	0.00%	0.01%	6.61%	0.10%	4.28%	0.35%	86.83%	1.63%	0.00%	0.07%	0.14%
68	5.095	5.30E-02	0.01%	0.00%	92.80%	2.17%	0.01%	3.80%	0.08%	0.00%	0.00%	0.00%	1.13%
69	5.108	0.00E+00	0.00%	0.00%	0.07%	0.00%	2.83%	0.01%	95.61%	1.44%	0.00%	0.04%	0.00%
70	5.126	1.00E-03	0.05%	0.00%	9.63%	1.12%	0.61%	83.48%	1.45%	0.04%	0.00%	0.02%	3.60%
71	5.151	0.00E+00	0.00%	0.00%	0.10%	0.01%	2.22%	0.07%	96.12%	1.44%	0.00%	0.03%	0.01%
72	5.180	1.00E-03	0.01%	0.00%	11.48%	0.35%	3.44%	2.87%	79.85%	1.58%	0.00%	0.08%	0.35%
73	5.183	0.00E+00	0.00%	0.00%	3.24%	0.09%	2.94%	0.65%	90.46%	2.45%	0.00%	0.08%	0.09%
74	5.193	2.00E-03	0.01%	0.00%	9.07%	0.46%	3.63%	3.95%	80.22%	2.36%	0.00%	0.10%	0.21%
75	5.205	1.00E-03	0.14%	0.01%	71.52%	6.60%	0.14%	16.20%	1.95%	0.09%	0.03%	0.00%	3.31%
76	5.216	6.90E-02	0.05%	0.00%	80.42%	7.56%	0.18%	6.25%	3.81%	0.13%	0.01%	0.01%	1.60%
77	5.230	1.00E-03	0.00%	0.00%	1.13%	0.10%	2.15%	0.23%	93.62%	2.68%	0.00%	0.06%	0.02%
78	5.259	4.80E-02	0.03%	0.00%	91.82%	1.63%	0.05%	2.02%	1.50%	0.08%	0.00%	0.00%	2.87%
79	5.262	1.00E-03	0.00%	0.00%	1.42%	0.04%	2.79%	0.43%	90.66%	4.47%	0.00%	0.14%	0.06%
80	5.270	0.00E+00	0.01%	0.00%	0.31%	0.06%	4.09%	5.10%	85.69%	4.26%	0.00%	0.21%	0.27%

Table S11: Energy (in Ev), oscillator strength and nature of the singlet states of 1-Pt

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
1	1.936	0.00E+00	3.15%	0.00%	4.95%	76.01%	0.05%	12.23%	0.01%	0.00%	1.86%	0.00%	1.75%
2	2.077	1.00E-03	2.88%	0.00%	4.19%	70.41%	0.05%	18.61%	0.01%	0.00%	1.76%	0.00%	2.10%
3	2.262	1.41E-01	1.58%	0.06%	11.25%	67.65%	1.20%	12.84%	0.64%	0.06%	2.42%	0.04%	2.26%
4	2.745	2.00E-03	0.03%	2.55%	6.40%	0.69%	52.95%	0.23%	32.49%	2.03%	0.03%	1.15%	1.46%
5	2.793	1.70E-02	2.81%	0.06%	4.70%	72.76%	0.63%	13.37%	0.39%	0.03%	3.32%	0.01%	1.92%
6	2.914	1.10E-02	2.49%	0.07%	6.01%	70.25%	1.08%	15.62%	0.08%	0.01%	2.45%	0.02%	1.93%
7	2.920	0.00E+00	2.45%	0.01%	11.29%	77.19%	0.22%	7.23%	0.03%	0.00%	0.66%	0.00%	0.91%
8	2.946	1.00E-03	5.02%	0.00%	10.74%	76.54%	0.04%	6.25%	0.02%	0.00%	0.22%	0.00%	1.16%
9	2.955	3.00E-03	0.03%	3.72%	3.29%	1.00%	84.07%	0.40%	3.93%	0.37%	0.05%	1.83%	1.31%
10	3.004	1.80E-02	1.27%	0.03%	8.79%	73.06%	1.38%	12.08%	0.80%	0.05%	1.41%	0.06%	1.08%
11	3.049	2.54E-01	1.30%	0.19%	8.83%	66.50%	5.17%	12.40%	3.05%	0.19%	1.13%	0.15%	1.10%
12	3.070	9.20E-02	2.28%	0.01%	19.16%	72.15%	0.18%	5.03%	0.19%	0.00%	0.14%	0.01%	0.86%
13	3.080	0.00E+00	0.01%	2.37%	3.86%	0.26%	37.61%	0.08%	49.77%	3.45%	0.00%	0.83%	1.75%
14	3.104	3.60E-02	0.19%	1.39%	9.97%	18.72%	37.79%	5.44%	22.41%	1.46%	0.05%	1.17%	1.41%
15	3.126	3.00E-02	2.59%	0.14%	9.32%	66.34%	3.57%	13.61%	2.65%	0.15%	0.40%	0.07%	1.17%
16	3.166	2.17E-01	4.23%	0.01%	13.67%	69.54%	0.25%	10.28%	0.15%	0.01%	0.30%	0.01%	1.55%
17	3.173	1.21E-01	1.98%	0.05%	12.16%	67.19%	1.88%	13.66%	1.35%	0.08%	0.50%	0.05%	1.10%
18	3.204	3.80E-02	1.03%	0.04%	12.15%	71.56%	0.53%	12.98%	0.30%	0.02%	0.62%	0.02%	0.76%
19	3.228	0.00E+00	0.06%	0.05%	1.73%	1.51%	1.48%	87.79%	0.99%	0.06%	0.02%	0.05%	6.26%
20	3.277	3.00E-03	0.02%	0.00%	1.38%	0.96%	0.01%	91.12%	0.01%	0.00%	0.04%	0.00%	6.46%
21	3.375	0.00E+00	0.00%	32.76%	1.24%	0.01%	13.72%	0.03%	7.66%	16.26%	0.01%	0.45%	27.86%
22	3.458	1.00E-03	3.21%	33.18%	1.24%	5.27%	14.00%	0.83%	2.63%	3.58%	8.51%	0.47%	27.10%
23	3.496	1.00E-03	8.76%	12.89%	1.76%	14.17%	6.20%	2.16%	1.29%	0.58%	23.04%	0.24%	28.91%
24	3.519	4.00E-03	0.44%	31.13%	1.18%	0.72%	11.80%	0.13%	7.17%	18.45%	0.98%	0.32%	27.69%
25	3.520	6.00E-03	2.46%	18.66%	4.54%	15.35%	6.92%	2.36%	2.88%	7.63%	10.10%	0.22%	28.88%
26	3.559	2.60E-02	1.79%	5.28%	14.11%	57.41%	2.08%	8.27%	1.03%	2.49%	0.73%	0.06%	6.77%
27	3.607	5.00E-03	10.16%	0.24%	2.27%	15.60%	5.32%	3.44%	3.59%	0.34%	27.94%	0.24%	30.87%
28	3.631	5.60E-02	1.17%	5.23%	5.14%	2.36%	41.43%	0.79%	30.29%	2.47%	3.00%	1.82%	6.31%
29	3.697	1.00E-03	6.99%	10.27%	2.55%	13.42%	3.96%	2.34%	1.72%	4.08%	22.10%	0.10%	32.48%
30	3.727	0.00E+00	0.01%	0.08%	3.70%	0.02%	0.51%	0.08%	88.64%	5.77%	0.01%	0.01%	1.18%
31	3.793	3.00E-03	0.03%	0.86%	6.98%	0.36%	49.11%	0.55%	38.51%	1.65%	0.01%	1.34%	0.60%

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
32	3.830	2.0E-03	1.08%	0.00%	16.79%	75.14%	0.08%	4.94%	0.03%	0.00%	0.86%	0.00%	1.06%
33	3.857	3.00E-03	0.01%	2.64%	3.18%	0.07%	84.81%	0.17%	4.16%	0.40%	0.00%	3.96%	0.59%
34	3.940	0.00E+00	0.00%	1.24%	3.72%	0.02%	37.59%	0.17%	50.99%	3.93%	0.00%	1.71%	0.63%
35	3.974	3.00E-03	44.96%	0.15%	4.43%	29.60%	0.69%	2.85%	0.41%	0.08%	3.99%	0.02%	12.83%
36	3.980	3.30E-02	5.29%	0.01%	18.99%	65.73%	0.36%	4.50%	0.19%	0.01%	1.94%	0.01%	2.98%
37	3.986	2.35E-01	1.02%	1.89%	7.30%	1.81%	46.36%	4.52%	32.15%	1.97%	0.04%	1.22%	1.72%
38	4.006	1.00E-03	0.39%	0.07%	18.88%	12.48%	1.69%	60.64%	1.27%	0.09%	0.09%	0.05%	4.35%
39	4.012	6.00E-03	32.29%	0.16%	6.00%	27.47%	7.03%	2.94%	3.90%	0.11%	6.83%	0.11%	13.17%
40	4.016	6.80E-02	4.11%	0.74%	10.27%	5.32%	47.70%	1.02%	26.53%	0.67%	0.80%	0.65%	2.20%
41	4.025	1.00E-03	0.03%	0.97%	3.28%	0.25%	86.57%	0.12%	7.10%	0.19%	0.02%	1.15%	0.33%
42	4.035	0.00E+00	3.45%	0.06%	12.75%	71.73%	1.48%	8.47%	1.00%	0.06%	0.07%	0.04%	0.89%
43	4.044	8.00E-03	0.91%	0.03%	18.93%	50.03%	0.70%	25.55%	0.48%	0.03%	0.06%	0.02%	3.24%
44	4.059	4.70E-02	0.20%	0.00%	8.60%	2.76%	0.06%	82.12%	0.06%	0.01%	0.07%	0.00%	6.12%
45	4.106	0.00E+00	0.04%	0.59%	4.65%	0.08%	44.32%	0.05%	47.84%	1.34%	0.02%	0.59%	0.48%
46	4.111	9.00E-03	42.22%	0.01%	4.46%	25.44%	0.07%	4.56%	0.08%	0.02%	5.94%	0.02%	17.20%
47	4.141	1.40E-02	2.45%	0.01%	14.89%	75.51%	0.06%	5.83%	0.04%	0.01%	0.25%	0.00%	0.95%
48	4.143	5.00E-03	0.05%	0.08%	0.66%	0.25%	49.34%	7.02%	40.10%	1.01%	0.01%	1.23%	0.27%
49	4.165	9.80E-02	1.02%	0.00%	20.85%	69.74%	0.31%	6.93%	0.23%	0.01%	0.09%	0.01%	0.82%
50	4.167	4.70E-02	0.78%	0.00%	40.68%	51.89%	0.14%	4.87%	0.08%	0.00%	0.04%	0.00%	1.52%
51	4.177	2.13E-01	1.18%	0.00%	39.41%	46.82%	0.27%	9.32%	0.19%	0.00%	0.17%	0.01%	2.64%
52	4.214	0.00E+00	0.00%	0.00%	0.97%	0.02%	47.64%	6.37%	40.20%	2.04%	0.00%	2.41%	0.36%
53	4.229	7.00E-03	0.10%	0.00%	1.74%	3.58%	0.17%	91.47%	0.11%	0.00%	0.01%	0.00%	2.82%
54	4.235	1.35E-01	0.94%	0.00%	50.77%	38.87%	0.78%	5.94%	0.55%	0.02%	0.05%	0.02%	2.06%
55	4.257	1.97E-01	0.63%	0.00%	52.34%	37.39%	0.34%	7.02%	0.22%	0.00%	0.03%	0.01%	2.03%
56	4.271	1.44E-01	0.65%	0.00%	67.14%	23.39%	0.28%	5.39%	0.19%	0.01%	0.03%	0.02%	2.91%
57	4.277	2.30E-02	0.19%	0.00%	13.94%	5.65%	0.12%	76.41%	0.11%	0.01%	0.02%	0.00%	3.56%
58	4.283	1.40E-02	2.15%	0.00%	35.94%	39.39%	0.45%	19.54%	0.32%	0.01%	0.12%	0.01%	2.08%
59	4.287	2.00E-02	2.75%	0.00%	32.51%	48.43%	0.61%	13.12%	0.43%	0.01%	0.14%	0.01%	2.00%
60	4.356	5.00E-03	0.03%	0.08%	1.36%	1.12%	50.66%	9.49%	34.80%	0.87%	0.00%	1.25%	0.35%
61	4.373	4.21E-01	1.63%	0.00%	46.25%	44.04%	0.18%	5.46%	0.13%	0.01%	0.07%	0.01%	2.22%
62	4.374	1.15E+00	1.21%	0.00%	40.79%	51.07%	0.48%	4.47%	0.29%	0.02%	0.03%	0.02%	1.63%
63	4.426	2.00E-02	0.07%	0.00%	1.35%	1.03%	49.66%	9.27%	33.82%	1.72%	0.00%	2.52%	0.55%
64	4.450	1.00E-03	0.01%	0.06%	0.05%	0.05%	76.42%	2.90%	18.10%	0.45%	0.00%	1.80%	0.11%
65	4.492	3.08E-01	0.02%	0.11%	26.52%	0.20%	29.97%	6.04%	32.64%	1.26%	0.00%	0.74%	2.52%
66	4.495	3.52E-01	0.02%	0.25%	29.64%	0.23%	28.39%	6.38%	30.26%	1.26%	0.00%	0.68%	2.89%
67	4.520	1.00E-03	0.19%	0.00%	0.32%	1.12%	73.89%	2.91%	16.73%	0.87%	0.01%	3.75%	0.22%
68	4.531	4.30E-02	6.27%	0.01%	13.70%	60.79%	1.45%	10.35%	1.75%	1.56%	0.37%	0.06%	3.69%
69	4.548	1.00E-03	0.00%	0.04%	3.37%	0.06%	2.99%	0.34%	83.14%	8.34%	0.00%	0.12%	1.60%
70	4.564	0.00E+00	0.22%	0.00%	0.17%	0.30%	49.96%	4.44%	40.06%	2.07%	0.00%	2.51%	0.29%
71	4.569	1.00E-03	44.74%	0.00%	5.64%	30.83%	0.21%	4.74%	0.25%	0.03%	0.86%	0.04%	12.67%
72	4.574	4.00E-03	45.29%	0.00%	5.05%	31.00%	0.10%	4.41%	0.08%	0.03%	1.40%	0.02%	12.62%
73	4.583	1.80E-02	0.38%	0.24%	1.32%	1.98%	0.30%	0.59%	20.89%	48.01%	0.02%	0.01%	26.26%
74	4.608	0.00E+00	0.44%	0.00%	2.53%	0.94%	0.03%	89.05%	0.25%	0.18%	0.01%	0.00%	6.58%
75	4.649	5.00E-03	0.11%	0.17%	4.24%	1.12%	3.86%	69.54%	8.68%	0.55%	0.04%	0.10%	11.58%
76	4.650	2.00E-03	0.79%	0.02%	1.63%	0.81%	0.35%	24.02%	0.79%	0.05%	0.20%	0.01%	71.32%
77	4.670	1.00E-03	24.71%	0.01%	6.18%	19.60%	0.11%	35.87%	0.38%	0.15%	0.85%	0.02%	12.13%
78	4.705	7.00E-03	0.01%	0.00%	1.15%	0.25%	0.01%	19.19%	0.01%	0.01%	0.62%	0.00%	78.76%
79	4.711	3.00E-03	16.73%	0.00%	6.76%	19.42%	0.13%	47.35%	0.38%	0.03%	0.36%	0.01%	8.82%
80	4.726	3.70E-02	0.13%	0.24%	10.63%	1.27%	5.10%	67.21%	9.06%	0.56%	0.03%	0.11%	5.67%

*Table S12: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Au(I)***

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
1	2.166	0.00E+00	3.35%	0.00%	5.47%	77.10%	0.06%	11.86%	0.02%	0.00%	1.04%	0.00%	1.10%
2	2.323	2.00E-03	2.76%	0.00%	4.89%	69.83%	0.07%	20.03%	0.03%	0.00%	0.94%	0.00%	1.45%
3	2.500	1.45E-01	1.63%	0.02%	12.09%	70.35%	0.38%	12.87%	0.13%	0.01%	1.24%	0.01%	1.28%
4	2.806	2.10E-02	2.24%	0.01%	6.87%	77.46%	0.13%	11.18%	0.04%	0.00%	1.18%	0.00%	0.90%
5	2.824	1.00E-03	2.72%	0.00%	12.27%	78.23%	0.04%	6.03%	0.02%	0.00%	0.07%	0.00%	0.63%
6	2.848	2.00E-03	4.66%	0.00%	10.56%	77.33%	0.05%	6.21%	0.02%	0.00%	0.17%	0.00%	1.01%
7	2.953	4.00E-03	1.66%	0.25%	11.21%	55.26%	11.57%	15.19%	2.13%	0.09%	1.01%	0.26%	1.39%
8	2.961	3.00E-03	0.35%	0.87%	24.23%	15.72%	42.85%	4.97%	7.81%	0.36%	0.31%	1.05%	1.49%
9	2.980	1.05E-01	1.97%	0.00%	20.23%	71.23%	0.11%	5.69%	0.03%	0.00%	0.01%	0.00%	0.72%
10	3.020	4.70E-02	0.96%	0.00%	13.51%	72.20%	0.14%	12.43%	0.03%	0.00%	0.28%	0.00%	0.46%
11	3.070	2.06E-01	4.17%	0.00%	14.54%	69.71%	0.09%	9.51%	0.03%	0.00%	0.41%	0.01%	1.54%
12	3.083	1.37E-01	4.02%	0.00%	13.97%	70.03%	0.11%	10.27%	0.03%	0.00%	0.19%	0.01%	1.37%
13	3.236	5.70E-02	2.04%	0.00%	9.00%	76.07%	0.08%	11.88%	0.02%	0.00%	0.20%	0.00%	0.71%
14	3.378	2.60E-02	0.99%	0.00%	7.82%	71.68%	0.11%	18.72%	0.04%	0.00%	0.15%	0.00%	0.49%
15	3.443	4.80E-02	1.11%	0.00%	10.95%	73.31%	0.17%	13.86%	0.04%	0.00%	0.10%	0.00%	0.46%
16	3.555	8.00E-02	1.13%	0.01%	10.98%	55.76%	0.36%	29.81%	0.07%	0.00%	0.11%	0.02%	1.76%
17	3.583	3.00E-03	0.38%	0.02%	4.77%	15.75%	0.75%	74.03%	0.47%	0.03%	0.02%	0.03%	3.77%
18	3.613	2.00E-03	0.04%	1.03%	25.21%	1.31%	57.92%	1.50%	9.14%	0.49%	0.01%	1.86%	1.51%
19	3.628	5.00E-03	0.05%	0.01%	2.09%	1.01%	0.19%	91.92%	0.16%	0.01%	0.01%	0.01%	4.56%
20	3.683	1.00E-03	0.00%	1.25%	3.23%	0.03%	52.34%	0.07%	39.59%	1.82%	0.00%	1.28%	0.39%
21	3.708	7.60E-02	0.06%	1.17%	5.78%	1.65%	40.05%	1.34%	45.98%	2.17%	0.01%	1.07%	0.72%
22	3.742	4.00E-03	1.73%	0.01%	14.73%	75.38%	0.53%	6.30%	0.59%	0.03%	0.13%	0.01%	0.56%
23	3.892	3.90E-02	7.76%	0.00%	18.18%	66.26%	0.04%	5.60%	0.02%	0.00%	0.23%	0.00%	1.89%
24	3.925	4.00E-03	13.62%	0.00%	12.64%	64.10%	0.08%	6.38%	0.03%	0.00%	0.24%	0.01%	2.92%
25	3.937	4.00E-03	34.02%	0.00%	9.33%	44.35%	0.07%	4.07%	0.02%	0.01%	0.57%	0.02%	7.56%
26	3.957	6.00E-03	21.16%	0.00%	14.17%	53.29%	0.09%	6.12%	0.03%	0.00%	0.23%	0.01%	4.90%
27	3.967	8.00E-03	28.82%	0.00%	9.92%	48.73%	0.17%	5.74%	0.04%	0.00%	0.22%	0.01%	6.35%
28	4.011	1.00E-03	0.05%	0.15%	34.44%	1.17%	51.11%	2.31%	9.37%	0.15%	0.00%	0.63%	0.63%
29	4.040	4.00E-03	6.49%	0.00%	14.18%	70.18%	0.44%	6.66%	0.11%	0.00%	0.11%	0.02%	1.82%
30	4.055	3.30E-02	0.41%	0.02%	7.88%	41.19%	27.62%	15.69%	5.68%	0.15%	0.01%	0.80%	0.55%
31	4.055	3.80E-02	0.90%	0.02%	7.78%	39.35%	28.33%	16.05%	5.82%	0.17%	0.02%	0.84%	0.74%
32	4.078	7.00E-03	45.18%	0.00%	5.87%	32.02%	0.29%	4.09%	0.06%	0.01%	0.44%	0.03%	12.01%
33	4.085	4.00E-03	2.33%	0.00%	28.68%	61.41%	0.21%	6.32%	0.06%	0.00%	0.03%	0.01%	0.95%
34	4.106	8.30E-02	1.74%	0.00%	28.65%	52.09%	0.61%	15.51%	0.16%	0.01%	0.05%	0.02%	1.17%
35	4.132	1.00E-03	0.18%	0.01%	0.89%	0.94%	56.23%	24.78%	11.88%	0.65%	0.00%	3.03%	1.42%
36	4.138	3.90E-02	0.46%	0.00%	17.85%	18.70%	0.08%	60.35%	0.03%	0.00%	0.01%	0.00%	2.51%
37	4.158	7.00E-03	0.03%	1.90%	11.72%	0.54%	76.23%	0.71%	6.10%	0.31%	0.00%	1.73%	0.74%
38	4.162	1.58E-01	1.16%	0.01%	34.27%	52.33%	0.54%	10.66%	0.07%	0.00%	0.03%	0.01%	0.91%
39	4.182	1.00E-02	3.64%	0.00%	13.40%	69.24%	0.26%	12.17%	0.09%	0.00%	0.03%	0.01%	1.18%

			M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
40	4.190	5.00E-02	0.92%	0.00%	26.78%	42.83%	0.10%	26.51%	0.03%	0.00%	0.02%	0.00%	2.82%
41	4.228	7.50E-02	0.56%	0.03%	14.71%	17.62%	0.85%	62.54%	0.81%	0.04%	0.01%	0.03%	2.82%
42	4.257	1.05E-01	0.59%	0.00%	67.02%	15.99%	0.11%	12.62%	0.08%	0.01%	0.01%	0.01%	3.56%
43	4.280	6.00E-03	0.05%	0.02%	84.46%	0.94%	0.88%	7.96%	0.98%	0.05%	0.00%	0.03%	4.63%
44	4.284	1.00E-03	0.00%	0.76%	3.00%	0.03%	50.89%	0.18%	41.09%	2.02%	0.00%	1.78%	0.26%
45	4.288	9.00E-03	0.01%	2.48%	2.60%	0.10%	92.09%	0.13%	0.16%	0.02%	0.00%	1.98%	0.44%
46	4.291	8.40E-02	0.02%	1.21%	7.57%	0.47%	40.01%	2.71%	43.75%	2.10%	0.00%	1.26%	0.90%
47	4.323	1.58E+00	0.76%	0.00%	61.53%	25.70%	0.07%	8.39%	0.06%	0.00%	0.01%	0.00%	3.47%
48	4.339	3.90E-01	0.52%	0.00%	76.45%	14.43%	0.04%	4.18%	0.02%	0.00%	0.01%	0.00%	4.36%
49	4.492	2.30E-02	8.43%	0.03%	14.01%	61.79%	0.49%	10.18%	0.30%	0.03%	0.76%	0.06%	3.93%
50	4.516	3.00E-03	42.84%	0.01%	5.21%	30.50%	0.11%	4.04%	0.03%	0.01%	3.70%	0.02%	13.53%
51	4.573	3.00E-03	43.13%	0.01%	5.59%	29.42%	0.75%	7.46%	0.84%	0.03%	0.88%	0.05%	11.84%
52	4.596	9.00E-03	1.47%	0.00%	4.35%	2.29%	0.48%	88.71%	0.61%	0.04%	0.04%	0.02%	2.00%
53	4.606	2.00E-03	1.05%	0.02%	0.88%	1.39%	36.41%	7.34%	50.22%	1.26%	0.03%	0.93%	0.48%
54	4.674	2.10E-02	1.92%	0.01%	6.28%	2.25%	0.28%	86.60%	0.33%	0.02%	0.07%	0.02%	2.22%
55	4.676	3.00E-03	0.00%	0.02%	0.49%	0.02%	47.01%	2.25%	47.79%	1.13%	0.00%	1.19%	0.10%
56	4.683	5.10E-02	4.14%	0.05%	5.66%	3.39%	30.58%	7.28%	42.77%	2.34%	0.18%	1.66%	1.96%
57	4.687	5.91E-01	6.05%	0.52%	54.97%	5.91%	7.97%	7.20%	10.55%	0.56%	0.26%	0.38%	5.64%
58	4.688	1.88E-01	29.69%	0.14%	21.70%	21.36%	2.25%	9.52%	2.92%	0.16%	1.29%	0.10%	10.87%
59	4.737	1.40E-02	0.14%	1.37%	38.50%	1.37%	41.65%	6.37%	7.20%	0.41%	0.05%	0.59%	2.37%
60	4.753	0.00E+00	0.01%	0.00%	0.04%	0.02%	47.31%	2.30%	45.09%	2.48%	0.00%	2.61%	0.13%
61	4.755	3.60E-02	0.01%	0.20%	9.12%	0.44%	40.52%	1.20%	46.55%	0.98%	0.01%	0.66%	0.31%
62	4.807	1.00E-03	0.00%	0.22%	2.86%	0.02%	52.54%	0.16%	42.26%	0.89%	0.00%	0.97%	0.08%
63	4.818	3.00E-03	0.03%	0.54%	15.34%	0.60%	70.63%	2.97%	5.68%	0.25%	0.02%	3.20%	0.74%
64	4.869	1.00E-03	1.68%	0.02%	6.56%	63.71%	2.12%	18.04%	0.69%	0.02%	3.94%	0.06%	3.17%
65	4.889	0.00E+00	0.10%	0.19%	1.60%	2.21%	56.49%	24.29%	12.85%	0.21%	0.51%	0.73%	0.81%
66	4.900	8.00E-03	0.07%	1.20%	8.60%	4.06%	79.64%	1.94%	0.64%	0.05%	0.20%	2.91%	0.69%
67	4.923	2.00E-03	3.20%	0.17%	2.19%	24.25%	0.64%	7.38%	0.12%	0.07%	38.83%	0.03%	23.11%
68	4.947	1.20E-02	0.61%	0.21%	8.88%	20.68%	2.40%	60.75%	0.29%	0.07%	1.77%	0.10%	4.25%
69	4.952	2.10E-02	0.80%	0.65%	10.75%	38.96%	6.14%	38.39%	0.59%	0.20%	0.57%	0.25%	2.71%
70	4.970	3.90E-02	1.40%	0.57%	11.24%	55.92%	3.31%	20.67%	0.56%	0.18%	2.84%	0.12%	3.19%
71	5.009	1.20E-02	0.13%	1.24%	5.65%	6.03%	0.78%	78.98%	0.89%	0.38%	0.54%	0.03%	5.33%
72	5.035	2.70E-02	1.07%	2.70%	15.00%	7.84%	2.75%	38.37%	1.11%	0.90%	14.91%	0.08%	15.27%
73	5.038	1.50E-02	1.04%	3.37%	44.54%	7.92%	3.09%	14.66%	1.09%	1.15%	10.83%	0.14%	12.16%
74	5.046	3.00E-02	0.69%	1.48%	47.44%	5.73%	1.37%	29.77%	0.98%	0.56%	4.77%	0.08%	7.13%
75	5.058	5.00E-03	0.65%	3.42%	1.83%	4.22%	40.78%	21.17%	8.58%	1.18%	8.64%	0.61%	8.94%
76	5.060	4.00E-03	4.79%	0.56%	6.05%	16.38%	2.32%	7.18%	0.64%	0.34%	34.67%	0.04%	27.05%
77	5.082	5.00E-03	0.47%	14.30%	8.73%	3.99%	17.10%	24.67%	4.88%	4.65%	5.05%	0.57%	15.60%
78	5.096	8.40E-02	0.10%	3.88%	64.37%	2.88%	3.33%	16.66%	1.10%	1.26%	1.01%	0.15%	5.26%
79	5.100	9.00E-03	0.12%	1.21%	42.55%	5.11%	2.29%	41.88%	1.72%	0.49%	0.23%	0.10%	4.29%
80	5.185	3.60E-02	0.17%	1.31%	46.36%	7.79%	5.24%	31.20%	3.37%	0.73%	0.20%	0.17%	3.47%

*Table S13: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Au(III)***

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
1	1.210	0.00E+00	0.63%	0.01%	1.34%	17.65%	0.00%	3.16%	0.00%	0.01%	31.44%	0.00%	45.76%
2	1.334	0.00E+00	0.64%	0.01%	0.98%	16.27%	0.01%	4.89%	0.00%	0.01%	28.96%	0.00%	48.24%
3	1.349	1.00E-03	0.49%	0.04%	2.92%	15.95%	0.02%	3.22%	0.03%	0.06%	28.47%	0.00%	48.79%
4	1.693	0.00E+00	3.71%	0.00%	4.88%	76.20%	0.02%	12.59%	0.01%	0.00%	1.15%	0.00%	1.44%
5	1.833	1.00E-03	3.25%	0.00%	4.05%	70.61%	0.02%	19.19%	0.01%	0.00%	1.09%	0.00%	1.77%
6	2.082	1.07E-01	1.67%	0.01%	11.91%	68.93%	0.07%	13.87%	0.12%	0.06%	1.53%	0.00%	1.83%
7	2.165	0.00E+00	0.01%	0.00%	0.23%	0.15%	0.00%	21.78%	0.00%	0.01%	0.27%	0.00%	77.55%
8	2.222	0.00E+00	0.02%	0.00%	0.24%	0.31%	0.00%	21.69%	0.00%	0.00%	0.54%	0.00%	77.20%
9	2.584	1.90E-02	3.63%	0.01%	4.79%	74.86%	0.03%	13.21%	0.03%	0.02%	1.94%	0.00%	1.49%
10	2.638	0.00E+00	0.00%	4.81%	0.73%	0.01%	2.68%	0.02%	18.74%	33.87%	0.01%	0.05%	39.08%
11	2.711	9.00E-03	3.29%	0.02%	4.41%	69.78%	0.02%	18.71%	0.05%	0.07%	1.77%	0.00%	1.89%
12	2.802	2.00E-03	0.01%	7.91%	0.79%	0.22%	4.29%	0.06%	16.85%	30.98%	0.01%	0.06%	38.83%
13	2.815	2.60E-02	0.02%	0.28%	0.87%	0.91%	0.15%	0.55%	20.54%	37.92%	0.01%	0.00%	38.76%
14	2.830	2.00E-03	1.95%	0.00%	6.93%	74.40%	0.03%	14.30%	0.20%	0.30%	0.66%	0.00%	1.23%
15	2.858	0.00E+00	0.00%	0.00%	1.36%	1.08%	0.00%	91.78%	0.07%	0.13%	0.04%	0.00%	5.53%
16	2.912	2.00E-03	0.03%	0.00%	1.31%	1.22%	0.00%	92.00%	0.00%	0.00%	0.03%	0.00%	5.40%
17	2.913	0.00E+00	0.02%	7.25%	0.86%	0.56%	3.94%	0.22%	16.90%	30.95%	0.08%	0.06%	39.17%
18	2.922	3.80E-02	2.02%	0.05%	6.18%	70.81%	0.06%	18.65%	0.17%	0.27%	0.49%	0.00%	1.29%
19	3.039	6.40E-02	1.54%	0.00%	12.89%	73.86%	0.03%	10.89%	0.03%	0.01%	0.16%	0.00%	0.60%
20	3.042	3.57E-01	1.55%	0.01%	10.32%	72.34%	0.02%	14.14%	0.09%	0.11%	0.44%	0.00%	0.99%
21	3.049	2.30E-02	1.75%	0.00%	12.97%	76.21%	0.02%	8.35%	0.02%	0.00%	0.10%	0.00%	0.56%
22	3.082	1.80E-02	4.47%	0.00%	12.26%	76.72%	0.02%	5.53%	0.02%	0.01%	0.02%	0.00%	0.97%
23	3.202	1.55E-01	1.73%	0.00%	21.72%	71.21%	0.02%	4.68%	0.02%	0.00%	0.01%	0.00%	0.61%
24	3.272	5.00E-03	2.63%	0.00%	16.27%	70.16%	0.04%	9.93%	0.06%	0.00%	0.02%	0.00%	0.89%
25	3.311	1.13E-01	3.96%	0.00%	13.92%	68.68%	0.04%	11.13%	0.05%	0.02%	0.01%	0.00%	2.19%
26	3.321	1.00E-03	0.04%	0.07%	19.64%	0.88%	0.04%	1.80%	0.66%	1.19%	0.15%	0.00%	75.54%
27	3.561	4.00E-03	0.00%	0.00%	0.35%	0.09%	0.00%	21.73%	0.02%	0.03%	0.14%	0.00%	77.64%
28	3.609	3.00E-03	2.45%	0.00%	16.56%	60.22%	0.02%	18.37%	0.02%	0.01%	0.09%	0.00%	2.28%
29	3.631	0.00E+00	0.04%	0.01%	0.64%	0.22%	0.01%	21.29%	0.02%	0.03%	0.37%	0.00%	77.37%
30	3.679	6.00E-03	0.06%	0.01%	0.89%	0.53%	0.01%	20.74%	0.04%	0.06%	0.90%	0.00%	76.76%
31	3.709	2.00E-03	0.38%	0.00%	4.83%	8.66%	0.01%	79.89%	0.01%	0.00%	0.04%	0.00%	6.18%
32	3.739	0.00E+00	0.56%	0.09%	1.42%	1.30%	0.05%	20.62%	0.07%	0.11%	1.81%	0.00%	73.98%
33	3.748	6.00E-03	0.11%	0.00%	3.23%	1.18%	0.00%	87.78%	0.00%	0.00%	0.06%	0.00%	7.63%
34	3.840	7.00E-03	0.07%	0.02%	0.53%	0.25%	0.01%	21.33%	0.07%	0.10%	0.40%	0.00%	77.23%
35	3.875	0.00E+00	46.37%	0.01%	5.17%	32.66%	0.02%	3.96%	0.02%	0.01%	0.26%	0.02%	11.50%
36	3.924	1.00E-03	0.18%	0.00%	0.94%	0.80%	0.00%	95.97%	0.01%	0.00%	0.00%	0.00%	2.09%
37	3.949	0.00E+00	52.85%	0.00%	4.15%	29.16%	0.01%	2.54%	0.03%	0.01%	0.11%	0.01%	11.15%
38	3.963	3.00E-03	7.30%	0.00%	18.56%	65.91%	0.02%	5.53%	0.01%	0.00%	0.06%	0.00%	2.61%
39	3.979	7.00E-03	0.02%	0.00%	0.75%	1.17%	0.00%	96.14%	0.01%	0.00%	0.00%	0.00%	1.91%
40	3.990	2.30E-02	0.08%	2.51%	5.72%	0.09%	10.79%	0.28%	72.39%	3.97%	0.01%	0.27%	3.90%
41	4.057	2.00E-03	39.87%	0.04%	4.07%	25.36%	0.05%	6.60%	0.25%	0.03%	0.52%	0.01%	23.20%
42	4.057	1.00E-02	3.87%	0.02%	0.97%	3.61%	0.02%	18.88%	0.11%	0.07%	2.14%	0.00%	70.32%
43	4.088	0.00E+00	0.00%	0.02%	4.25%	0.04%	0.62%	0.91%	88.95%	4.48%	0.00%	0.02%	0.73%
44	4.096	6.00E-03	3.53%	0.91%	4.17%	12.41%	0.57%	15.40%	0.82%	0.07%	3.27%	0.01%	58.84%
45	4.107	9.30E-02	0.79%	0.01%	62.31%	30.33%	0.02%	3.76%	0.02%	0.00%	0.06%	0.00%	2.70%
46	4.110	7.60E-02	3.89%	0.13%	24.88%	58.96%	0.09%	5.20%	0.07%	0.01%	0.39%	0.00%	6.39%
47	4.176	2.00E-03	1.96%	0.00%	14.77%	73.03%	0.04%	9.49%	0.05%	0.00%	0.07%	0.00%	0.59%

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
48	4.192	4.30E-02	0.03%	26.41%	5.38%	0.45%	15.12%	2.37%	9.26%	2.56%	0.29%	0.23%	37.90%
49	4.208	7.62E-01	0.88%	0.23%	73.31%	19.65%	0.14%	2.74%	0.07%	0.03%	0.02%	0.00%	2.94%
50	4.236	8.30E-02	1.12%	0.00%	51.73%	41.70%	0.02%	3.80%	0.03%	0.00%	0.02%	0.00%	1.59%
51	4.242	0.00E+00	0.00%	0.29%	3.40%	0.02%	13.36%	0.17%	77.64%	3.99%	0.00%	0.41%	0.72%
52	4.247	8.00E-03	0.06%	0.02%	2.77%	2.51%	0.62%	85.62%	3.11%	0.16%	0.01%	0.02%	5.11%
53	4.253	3.10E-02	0.09%	0.00%	92.64%	2.52%	0.00%	0.98%	0.00%	0.00%	0.00%	0.00%	3.77%
54	4.256	9.00E-03	2.36%	0.01%	18.50%	66.64%	0.24%	9.96%	0.99%	0.06%	0.05%	0.01%	1.19%
55	4.280	3.80E-02	0.49%	0.00%	61.62%	32.40%	0.01%	2.67%	0.02%	0.00%	0.02%	0.00%	2.77%
56	4.281	3.10E-02	0.05%	1.03%	8.45%	1.83%	0.57%	80.93%	0.36%	0.29%	0.03%	0.01%	6.47%
57	4.295	1.30E-02	0.34%	0.28%	6.43%	4.12%	10.85%	19.96%	51.70%	2.76%	0.04%	0.32%	3.19%
58	4.300	7.80E-02	0.57%	0.01%	14.83%	78.68%	0.02%	5.65%	0.02%	0.00%	0.01%	0.00%	0.22%
59	4.339	1.36E-01	2.85%	0.02%	28.74%	51.00%	0.75%	9.51%	4.22%	0.24%	0.10%	0.02%	2.55%
60	4.368	2.30E-02	0.21%	0.06%	6.19%	8.68%	2.01%	65.58%	11.52%	0.64%	0.07%	0.06%	4.98%
61	4.373	8.50E-02	0.06%	1.11%	21.08%	2.48%	0.64%	63.95%	0.91%	0.66%	0.09%	0.01%	9.02%
62	4.378	2.53E-01	1.11%	0.07%	19.05%	67.62%	0.08%	11.07%	0.08%	0.04%	0.07%	0.00%	0.83%
63	4.406	3.90E-02	11.74%	0.01%	13.25%	61.27%	0.04%	10.35%	0.05%	0.01%	0.04%	0.00%	3.25%
64	4.444	2.54E-01	0.35%	0.34%	9.61%	4.50%	0.42%	12.51%	1.57%	0.85%	1.60%	0.01%	68.22%
65	4.448	1.33E-01	8.17%	0.01%	19.83%	54.64%	0.10%	8.53%	0.51%	0.05%	0.23%	0.01%	7.92%
66	4.453	1.90E-02	0.10%	1.56%	10.59%	4.22%	0.92%	28.65%	0.98%	1.51%	1.26%	0.02%	50.20%
67	4.457	1.10E-01	0.16%	0.60%	18.09%	3.47%	0.38%	4.24%	0.56%	0.60%	0.68%	0.01%	71.22%
68	4.471	7.76E-01	2.50%	0.07%	26.10%	62.27%	0.06%	5.80%	0.07%	0.09%	0.06%	0.00%	2.98%
69	4.527	8.00E-03	9.68%	0.00%	10.14%	57.75%	0.04%	16.66%	0.25%	0.02%	0.30%	0.00%	5.15%
70	4.532	3.00E-03	0.47%	0.01%	5.06%	5.78%	0.31%	79.21%	2.43%	0.14%	0.10%	0.01%	6.48%
71	4.541	3.40E-01	0.35%	0.14%	44.74%	4.99%	0.17%	21.58%	2.26%	0.32%	0.67%	0.00%	24.78%
72	4.571	1.50E-02	30.98%	0.00%	8.60%	44.33%	0.02%	7.26%	0.04%	0.01%	0.18%	0.01%	8.57%
73	4.572	3.30E-02	36.68%	0.00%	7.93%	38.74%	0.02%	6.38%	0.02%	0.01%	0.20%	0.01%	10.01%
74	4.670	1.10E-02	5.19%	0.00%	5.90%	18.17%	0.04%	64.74%	0.16%	0.01%	0.15%	0.00%	5.63%
75	4.680	0.00E+00	34.41%	0.00%	5.64%	37.85%	0.02%	11.04%	0.03%	0.01%	0.21%	0.01%	10.77%
76	4.707	4.30E-02	7.93%	0.01%	6.02%	54.50%	0.03%	27.86%	0.08%	0.03%	0.28%	0.00%	3.28%
77	4.764	5.20E-02	0.88%	0.08%	14.88%	56.23%	0.61%	20.44%	2.34%	0.50%	0.38%	0.04%	3.62%
78	4.771	1.00E-03	0.75%	0.05%	5.66%	16.31%	0.20%	71.72%	0.25%	0.03%	0.20%	0.01%	4.82%
79	4.830	2.00E-03	0.09%	7.64%	10.70%	2.85%	4.26%	6.41%	2.33%	1.83%	1.42%	0.07%	62.42%
80	4.831	0.00E+00	2.20%	0.22%	14.93%	56.48%	0.35%	19.49%	1.34%	0.15%	0.29%	0.01%	4.53%

*Table S14: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Hg***

State	Energy	Oscillator	M$_{Ru}$C	M$_M$C	LC	M$_{Ru}$LCT	M$_M$LCT	LLCT	XLCT	XMCT	M$_{Ru}$M$_M$CT	M$_M$M$_{Ru}$CT	Other
1	2.204	0.00E+00	3.64%	0.00%	5.43%	77.94%	0.04%	11.80%	0.05%	0.00%	0.18%	0.00%	0.91%
2	2.346	1.00E-03	3.19%	0.00%	4.76%	71.76%	0.05%	18.86%	0.06%	0.00%	0.16%	0.00%	1.17%
3	2.550	1.52E-01	1.89%	0.01%	12.10%	71.93%	0.01%	12.77%	0.02%	0.01%	0.25%	0.00%	1.01%
4	2.813	3.00E-03	1.99%	0.00%	12.23%	79.80%	0.03%	5.49%	0.03%	0.00%	0.01%	0.00%	0.42%
5	2.851	1.00E-03	5.35%	0.00%	11.27%	76.91%	0.03%	5.29%	0.03%	0.00%	0.01%	0.00%	1.11%
6	2.943	2.30E-02	2.26%	0.00%	5.96%	78.35%	0.05%	12.02%	0.06%	0.00%	0.52%	0.00%	0.79%
7	2.965	1.20E-01	2.08%	0.00%	19.41%	72.56%	0.03%	5.20%	0.04%	0.00%	0.01%	0.00%	0.67%
8	3.016	3.00E-03	1.81%	0.00%	13.60%	73.30%	0.01%	10.65%	0.02%	0.00%	0.03%	0.00%	0.58%
9	3.054	7.00E-02	2.65%	0.00%	9.56%	71.69%	0.03%	14.74%	0.03%	0.00%	0.25%	0.00%	1.04%
10	3.096	9.40E-02	3.82%	0.00%	9.57%	70.65%	0.02%	14.32%	0.03%	0.00%	0.23%	0.00%	1.36%
11	3.140	2.11E-01	3.03%	0.00%	15.60%	71.12%	0.03%	8.78%	0.03%	0.00%	0.24%	0.00%	1.18%
12	3.174	7.00E-03	1.72%	0.00%	7.37%	77.91%	0.03%	12.22%	0.04%	0.00%	0.13%	0.00%	0.57%
13	3.301	2.40E-02	0.96%	0.00%	5.89%	72.85%	0.06%	18.77%	0.07%	0.00%	0.53%	0.00%	0.87%
14	3.355	1.00E-03	0.42%	0.02%	0.65%	7.65%	0.00%	1.37%	0.01%	0.03%	44.42%	0.00%	45.44%
15	3.393	1.07E-01	0.97%	0.00%	12.26%	73.20%	0.01%	13.11%	0.01%	0.00%	0.05%	0.00%	0.40%
16	3.480	0.00E+00	0.34%	0.03%	1.14%	10.42%	0.01%	2.64%	0.01%	0.05%	38.42%	0.00%	46.95%
17	3.493	0.00E+00	0.47%	0.00%	1.04%	6.16%	0.00%	1.19%	0.00%	0.01%	41.31%	0.00%	49.81%
18	3.545	9.40E-02	1.55%	0.01%	12.73%	64.76%	0.02%	13.59%	0.02%	0.01%	2.83%	0.00%	4.48%
19	3.624	6.00E-03	0.10%	0.00%	2.48%	3.14%	0.00%	90.71%	0.00%	0.00%	0.03%	0.00%	3.54%
20	3.673	4.00E-03	0.10%	0.00%	2.22%	1.58%	0.01%	92.55%	0.02%	0.00%	0.00%	0.00%	3.54%
21	3.737	6.00E-03	2.00%	0.00%	14.41%	76.31%	0.03%	6.54%	0.04%	0.00%	0.04%	0.00%	0.62%
22	3.881	4.00E-02	8.25%	0.00%	18.29%	66.60%	0.03%	4.92%	0.04%	0.00%	0.07%	0.00%	1.80%
23	3.931	1.00E-03	13.23%	0.00%	12.62%	64.71%	0.02%	6.49%	0.03%	0.00%	0.13%	0.00%	2.77%
24	3.936	4.00E-03	44.52%	0.00%	6.30%	36.37%	0.02%	3.36%	0.02%	0.02%	0.27%	0.02%	9.09%
25	3.946	0.00E+00	29.52%	0.00%	11.03%	49.12%	0.02%	3.80%	0.02%	0.00%	0.22%	0.00%	6.26%
26	3.955	1.20E-02	7.65%	0.00%	16.31%	65.82%	0.02%	8.21%	0.02%	0.00%	0.08%	0.00%	1.90%
27	4.043	4.00E-03	7.69%	0.00%	14.67%	69.75%	0.02%	5.87%	0.03%	0.00%	0.04%	0.00%	1.94%
28	4.055	3.10E-02	18.37%	0.00%	10.23%	60.54%	0.01%	5.86%	0.02%	0.00%	0.12%	0.00%	4.84%
29	4.070	5.40E-02	27.81%	0.00%	8.70%	51.66%	0.03%	4.42%	0.04%	0.00%	0.19%	0.00%	7.15%
30	4.077	1.00E-03	1.62%	0.00%	28.50%	64.58%	0.03%	4.49%	0.04%	0.00%	0.01%	0.00%	0.73%
31	4.101	6.50E-02	4.79%	0.00%	28.41%	55.76%	0.01%	9.06%	0.01%	0.00%	0.04%	0.00%	1.92%
32	4.164	1.20E-02	0.19%	0.06%	37.31%	1.77%	13.29%	1.81%	42.23%	1.45%	0.00%	0.39%	1.50%
33	4.172	1.19E-01	1.59%	0.00%	41.84%	44.60%	0.21%	10.10%	0.66%	0.03%	0.01%	0.01%	0.97%
34	4.174	1.35E-01	1.74%	0.00%	38.57%	50.31%	0.09%	7.99%	0.25%	0.01%	0.01%	0.00%	1.02%
35	4.186	2.10E-02	4.24%	0.00%	13.36%	69.52%	0.03%	11.46%	0.09%	0.00%	0.01%	0.00%	1.28%
36	4.240	9.30E-02	1.02%	0.00%	49.90%	34.91%	0.02%	12.78%	0.03%	0.00%	0.01%	0.00%	1.33%
37	4.266	9.50E-02	0.19%	0.00%	81.38%	8.23%	0.01%	7.73%	0.01%	0.00%	0.00%	0.00%	2.45%
38	4.295	2.00E-03	0.01%	0.00%	25.19%	1.76%	0.00%	68.27%	0.01%	0.00%	0.00%	0.00%	4.76%
39	4.305	9.79E-01	1.00%	0.00%	52.66%	20.32%	0.01%	22.57%	0.02%	0.00%	0.01%	0.00%	3.42%
40	4.315	3.00E-03	0.06%	0.02%	68.43%	1.68%	5.93%	4.78%	15.64%	0.54%	0.01%	0.18%	2.74%
41	4.347	4.08E-01	0.54%	0.00%	71.90%	12.85%	0.03%	9.84%	0.07%	0.00%	0.00%	0.00%	4.76%
42	4.357	5.84E-01	0.17%	0.00%	26.26%	6.28%	0.01%	62.49%	0.01%	0.00%	0.00%	0.00%	4.79%
43	4.481	1.00E-03	0.02%	0.04%	0.10%	0.00%	7.01%	0.04%	89.10%	3.01%	0.00%	0.20%	0.31%
44	4.501	2.00E-02	6.87%	0.04%	14.88%	63.01%	0.09%	10.68%	0.42%	0.20%	0.14%	0.01%	3.66%
45	4.514	0.00E+00	0.00%	0.03%	0.22%	0.00%	5.70%	0.02%	90.51%	3.03%	0.00%	0.16%	0.34%
46	4.516	1.00E-03	0.15%	0.00%	0.24%	0.13%	0.01%	9.77%	0.07%	0.01%	0.24%	0.00%	89.39%
47	4.537	3.00E-03	0.05%	0.00%	1.57%	0.40%	0.00%	94.75%	0.00%	0.00%	0.01%	0.00%	3.22%
48	4.558	3.00E-03	47.91%	0.00%	4.73%	30.04%	0.03%	4.28%	0.09%	0.00%	0.41%	0.00%	12.51%
49	4.566	0.00E+00	41.67%	0.00%	5.15%	27.73%	0.02%	6.95%	0.02%	0.02%	0.15%	0.02%	18.28%
50	4.570	0.00E+00	4.76%	0.02%	0.79%	3.20%	0.00%	8.93%	0.02%	0.09%	0.57%	0.00%	81.61%
51	4.588	3.00E-03	0.74%	0.00%	1.52%	2.55%	0.01%	90.98%	0.03%	0.01%	0.02%	0.00%	4.14%
52	4.681	4.00E-03	43.49%	0.05%	6.82%	30.81%	0.02%	4.69%	0.11%	0.32%	0.25%	0.01%	13.44%
53	4.704	8.01E-01	0.06%	0.29%	82.50%	0.90%	0.16%	6.04%	0.43%	1.55%	0.04%	0.00%	8.03%
54	4.713	1.00E-03	0.06%	3.62%	0.17%	0.06%	0.53%	0.03%	7.59%	52.87%	0.00%	0.01%	35.06%
55	4.721	3.50E-02	0.01%	3.80%	0.56%	0.01%	0.69%	0.04%	8.02%	52.05%	0.00%	0.02%	34.82%

33

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
56	4.736	1.19E-01	0.20%	5.97%	2.48%	0.83%	0.83%	0.30%	5.31%	38.50%	0.19%	0.01%	45.38%
57	4.817	1.40E-02	0.09%	0.14%	42.90%	0.75%	12.67%	2.59%	36.46%	1.89%	0.00%	0.38%	2.11%
58	4.871	1.00E-03	1.56%	0.01%	18.33%	57.24%	1.98%	13.91%	5.23%	0.10%	0.13%	0.05%	1.48%
59	4.909	1.00E-03	0.39%	0.03%	46.02%	16.67%	6.90%	7.63%	19.60%	0.31%	0.04%	0.14%	2.29%
60	4.948	7.00E-03	0.59%	0.02%	11.76%	21.21%	2.33%	16.68%	44.49%	1.72%	0.04%	0.06%	1.11%
61	4.953	3.80E-02	0.50%	0.95%	12.99%	33.59%	0.16%	10.70%	2.79%	18.31%	0.14%	0.00%	19.88%
62	4.965	1.80E-02	1.29%	0.01%	10.60%	47.81%	1.27%	13.31%	23.62%	0.91%	0.09%	0.04%	1.07%
63	4.971	1.88E-01	0.41%	1.03%	17.51%	27.30%	0.16%	5.92%	3.30%	21.95%	0.13%	0.00%	22.28%
64	5.004	1.00E-03	0.07%	0.00%	10.23%	2.22%	0.14%	82.30%	2.02%	0.08%	0.00%	0.01%	2.93%
65	5.040	3.60E-02	0.02%	0.00%	86.29%	1.68%	0.02%	10.36%	0.16%	0.01%	0.00%	0.00%	1.46%
66	5.046	4.40E-02	0.09%	0.02%	10.38%	4.04%	0.59%	73.63%	7.11%	0.64%	0.01%	0.02%	3.47%
67	5.077	0.00E+00	0.02%	0.03%	17.05%	0.45%	5.98%	15.02%	58.01%	1.88%	0.00%	0.19%	1.38%
68	5.092	5.80E-02	0.02%	0.00%	86.55%	2.56%	0.02%	9.43%	0.11%	0.00%	0.00%	0.00%	1.31%
69	5.092	2.00E-03	0.15%	0.00%	13.87%	3.56%	0.52%	74.36%	4.01%	0.14%	0.00%	0.02%	3.37%
70	5.136	3.00E-03	0.14%	0.00%	20.53%	5.41%	0.65%	66.24%	3.62%	0.12%	0.01%	0.03%	3.24%
71	5.141	0.00E+00	0.01%	0.00%	5.59%	0.60%	12.07%	30.54%	48.78%	1.39%	0.00%	0.26%	0.76%
72	5.165	0.00E+00	0.00%	0.05%	0.06%	0.00%	6.89%	0.06%	89.73%	2.85%	0.00%	0.17%	0.20%
73	5.193	0.00E+00	0.00%	0.05%	0.29%	0.02%	5.93%	0.15%	90.12%	3.01%	0.00%	0.15%	0.28%
74	5.201	1.80E-02	0.07%	0.01%	62.14%	5.83%	0.60%	26.91%	2.88%	0.27%	0.00%	0.02%	1.28%
75	5.215	2.00E-03	0.26%	0.00%	58.32%	8.22%	3.31%	14.10%	13.30%	0.70%	0.00%	0.17%	1.61%
76	5.230	1.00E-03	0.04%	0.02%	32.03%	1.54%	9.27%	13.97%	40.96%	0.85%	0.00%	0.16%	1.16%
77	5.235	1.00E-03	0.08%	0.01%	26.58%	3.05%	9.60%	15.46%	40.84%	2.17%	0.00%	0.51%	1.72%
78	5.242	6.80E-02	0.05%	0.01%	65.91%	4.45%	0.12%	26.60%	0.51%	0.15%	0.00%	0.01%	2.19%
79	5.253	6.70E-02	0.02%	0.02%	57.30%	2.96%	0.04%	36.73%	0.22%	0.27%	0.01%	0.00%	2.44%
80	5.271	0.00E+00	0.02%	0.03%	9.22%	0.44%	0.05%	3.37%	0.28%	0.02%	0.51%	0.00%	86.07%

*Table S15: Energy (in Ev), oscillator strength and nature of the singlet states of **1-Pb***

State	Energy	Oscillator	$M_{Ru}C$	M_MC	LC	$M_{Ru}LCT$	M_MLCT	LLCT	XLCT	XMCT	$M_{Ru}M_MCT$	$M_MM_{Ru}CT$	Other
1	2.151	2.00E-03	3.35%	0.00%	5.60%	77.29%	0.06%	11.74%	0.04%	0.00%	0.68%	0.00%	1.23%
2	2.308	3.00E-03	2.97%	0.00%	4.73%	70.57%	0.08%	19.44%	0.02%	0.00%	0.64%	0.00%	1.56%
3	2.490	1.36E-01	1.81%	0.01%	11.93%	70.86%	0.02%	12.87%	0.09%	0.01%	0.90%	0.00%	1.50%
4	2.833	3.00E-03	2.17%	0.00%	12.71%	78.38%	0.04%	6.04%	0.03%	0.00%	0.05%	0.00%	0.57%
5	2.870	1.00E-03	4.95%	0.00%	11.80%	75.90%	0.04%	6.06%	0.04%	0.00%	0.03%	0.00%	1.17%
6	2.904	2.90E-02	2.26%	0.00%	5.89%	75.98%	0.07%	13.00%	0.05%	0.01%	1.19%	0.00%	1.56%
7	2.994	1.03E-01	2.38%	0.00%	19.60%	70.85%	0.05%	6.15%	0.03%	0.00%	0.06%	0.00%	0.89%
8	3.042	1.30E-02	1.74%	0.00%	10.39%	71.09%	0.03%	14.98%	0.05%	0.00%	0.54%	0.00%	1.17%
9	3.044	2.30E-02	1.49%	0.00%	10.88%	71.78%	0.04%	14.33%	0.05%	0.00%	0.43%	0.00%	1.01%
10	3.098	1.53E-01	4.53%	0.00%	12.48%	70.03%	0.02%	11.12%	0.06%	0.00%	0.17%	0.00%	1.59%
11	3.125	1.70E-01	3.40%	0.00%	14.47%	70.20%	0.03%	9.38%	0.08%	0.01%	0.69%	0.00%	1.75%
12	3.165	4.90E-02	1.80%	0.00%	7.96%	76.83%	0.06%	12.48%	0.05%	0.00%	0.15%	0.00%	0.68%
13	3.313	3.40E-02	1.01%	0.00%	6.65%	71.54%	0.08%	20.07%	0.03%	0.00%	0.12%	0.00%	0.51%
14	3.383	9.10E-02	1.00%	0.00%	11.77%	73.24%	0.01%	13.24%	0.12%	0.00%	0.13%	0.00%	0.49%
15	3.522	9.00E-03	0.10%	0.01%	3.40%	4.56%	0.96%	82.46%	3.95%	0.17%	0.02%	0.03%	4.34%
16	3.558	6.50E-02	1.58%	0.00%	12.27%	58.88%	0.25%	23.91%	1.05%	0.06%	0.19%	0.01%	1.80%
17	3.596	1.30E-02	0.23%	0.01%	3.96%	8.27%	0.32%	81.81%	1.04%	0.05%	0.03%	0.01%	4.29%
18	3.739	4.00E-03	2.21%	0.06%	15.26%	61.76%	3.81%	5.76%	9.49%	0.41%	0.25%	0.10%	0.91%
19	3.748	6.00E-03	0.41%	0.25%	14.69%	13.59%	16.96%	7.58%	42.65%	1.87%	0.07%	0.48%	1.45%
20	3.883	2.10E-02	23.78%	0.01%	11.86%	51.68%	0.04%	4.32%	0.03%	0.01%	2.32%	0.02%	5.96%
21	3.911	1.90E-02	29.37%	0.01%	10.38%	44.78%	0.03%	3.71%	0.02%	0.02%	3.75%	0.01%	7.92%
22	3.931	6.00E-03	24.56%	0.00%	9.74%	53.35%	0.02%	6.14%	0.04%	0.01%	0.82%	0.01%	5.31%
23	3.949	0.00E+00	8.43%	0.00%	17.37%	66.03%	0.05%	5.14%	0.07%	0.00%	0.67%	0.00%	2.25%
24	3.969	8.00E-03	13.51%	0.00%	14.66%	60.22%	0.03%	7.62%	0.10%	0.01%	0.54%	0.00%	3.30%
25	4.017	2.00E-03	0.05%	0.02%	1.20%	0.13%	0.74%	1.15%	91.88%	4.10%	0.01%	0.02%	0.72%
26	4.050	6.00E-03	26.78%	0.00%	8.64%	48.12%	0.02%	5.18%	0.24%	0.02%	2.62%	0.01%	8.37%
27	4.056	6.00E-03	21.71%	0.00%	10.39%	53.93%	0.02%	5.33%	0.05%	0.01%	2.06%	0.00%	6.50%
28	4.073	6.60E-02	2.96%	0.00%	13.39%	75.42%	0.05%	6.34%	0.07%	0.00%	0.73%	0.00%	1.04%
29	4.099	1.60E-02	1.10%	0.00%	31.10%	60.29%	0.08%	6.06%	0.24%	0.01%	0.24%	0.00%	0.89%
30	4.124	9.00E-02	1.28%	0.00%	32.83%	51.49%	0.07%	8.68%	3.88%	0.19%	0.28%	0.00%	1.29%
31	4.127	7.00E-03	0.09%	0.01%	5.60%	2.77%	0.73%	2.34%	83.69%	3.81%	0.02%	0.02%	0.93%
32	4.167	1.09E-01	1.29%	0.00%	37.88%	36.96%	0.17%	20.81%	1.59%	0.05%	0.20%	0.00%	1.06%
33	4.177	1.74E-01	1.64%	0.00%	33.79%	53.23%	0.04%	9.40%	0.06%	0.00%	0.59%	0.00%	1.24%
34	4.191	5.00E-03	3.86%	0.00%	14.63%	68.72%	0.01%	11.31%	0.09%	0.01%	0.16%	0.00%	1.21%
35	4.228	1.00E-03	0.79%	0.01%	10.57%	26.79%	0.52%	53.51%	2.31%	0.14%	0.89%	0.02%	4.46%
36	4.252	6.30E-02	0.49%	0.00%	68.39%	11.05%	0.25%	13.42%	1.50%	0.09%	0.50%	0.01%	4.29%
37	4.254	6.10E-02	0.74%	0.01%	35.91%	12.99%	0.39%	42.12%	2.40%	0.12%	1.79%	0.02%	3.53%
38	4.274	2.00E-03	0.13%	0.04%	5.39%	0.68%	2.31%	1.10%	84.84%	3.79%	0.58%	0.06%	1.08%
39	4.281	2.40E-02	6.63%	0.02%	10.56%	13.66%	0.06%	2.40%	1.82%	0.14%	45.87%	0.00%	18.84%
40	4.289	5.10E-02	0.33%	0.01%	45.87%	4.09%	0.18%	37.57%	0.74%	0.04%	3.83%	0.01%	7.34%
41	4.332	1.03E+00	1.77%	0.02%	51.89%	20.15%	0.29%	7.45%	1.40%	0.14%	8.80%	0.02%	8.08%
42	4.340	7.48E-01	0.83%	0.00%	67.66%	19.71%	0.03%	5.22%	0.15%	0.01%	1.62%	0.00%	4.77%
43	4.356	4.00E-03	0.11%	0.05%	22.42%	0.76%	2.05%	2.11%	66.97%	3.15%	0.39%	0.07%	1.92%
44	4.373	1.37E-01	7.18%	0.02%	12.33%	19.25%	0.08%	3.17%	1.07%	0.11%	36.14%	0.00%	20.64%
45	4.435	1.10E-02	9.56%	0.03%	2.66%	15.18%	0.13%	2.75%	0.34%	0.04%	45.07%	0.01%	24.23%
46	4.442	2.00E-03	0.10%	0.42%	13.44%	1.01%	19.13%	9.73%	50.17%	2.89%	0.44%	0.63%	2.05%
47	4.488	6.00E-03	0.52%	0.03%	3.91%	4.57%	1.86%	80.10%	6.12%	0.21%	0.57%	0.05%	2.07%
48	4.502	2.30E-02	7.37%	0.01%	11.39%	49.92%	0.24%	15.31%	1.02%	0.06%	7.72%	0.01%	6.95%
49	4.560	3.00E-03	0.49%	0.00%	2.32%	1.09%	0.38%	92.13%	1.31%	0.02%	0.36%	0.01%	1.88%
50	4.571	0.00E+00	34.80%	0.01%	5.81%	28.78%	0.08%	4.80%	0.19%	0.03%	10.68%	0.02%	14.81%
51	4.588	4.00E-03	35.96%	0.00%	5.56%	26.47%	0.06%	4.19%	0.16%	0.03%	12.47%	0.02%	15.08%
52	4.630	6.07E-01	0.75%	0.06%	72.25%	1.96%	2.28%	8.55%	8.14%	0.40%	0.43%	0.05%	5.15%
53	4.689	1.90E-02	0.17%	0.05%	13.64%	0.54%	20.24%	8.35%	54.05%	1.51%	0.04%	0.53%	0.89%
54	4.697	6.00E-03	7.33%	0.04%	4.17%	6.49%	1.88%	2.29%	67.08%	3.82%	2.47%	0.05%	4.39%
55	4.700	2.00E-02	23.65%	0.02%	8.53%	19.10%	1.17%	4.91%	21.04%	1.16%	8.17%	0.05%	12.21%
56	4.707	1.60E-02	1.10%	0.06%	9.44%	1.65%	19.98%	9.05%	55.06%	1.38%	0.79%	0.36%	1.14%
57	4.721	1.37E-01	1.84%	0.08%	34.95%	4.33%	5.84%	9.62%	35.14%	1.76%	2.07%	0.18%	4.19%
58	4.727	4.60E-02	3.94%	0.06%	6.28%	15.33%	0.57%	3.70%	2.25%	0.14%	44.07%	0.02%	23.65%
59	4.795	4.00E-03	0.02%	0.01%	1.57%	0.36%	21.13%	9.94%	61.74%	3.16%	0.24%	1.07%	0.75%
60	4.804	2.00E-03	0.02%	0.02%	4.83%	0.14%	0.94%	1.59%	86.13%	5.02%	0.00%	0.04%	1.26%
61	4.837	4.00E-03	3.14%	0.02%	2.55%	31.36%	0.07%	8.66%	0.12%	0.02%	32.99%	0.00%	21.08%
62	4.860	0.00E+00	5.63%	0.02%	4.13%	27.51%	0.08%	5.48%	0.38%	0.05%	33.40%	0.00%	23.31%
63	4.904	1.60E-02	2.96%	0.03%	7.46%	22.14%	0.62%	38.12%	3.65%	0.17%	13.68%	0.02%	11.16%

64	4.910	8.00E-03	0.73%	0.01%	3.91%	6.62%	1.18%	17.54%	63.02%	2.51%	2.11%	0.04%	2.35%
65	4.913	2.10E-02	1.40%	0.02%	6.10%	12.16%	1.39%	28.02%	41.22%	1.53%	3.93%	0.04%	4.21%
66	4.930	1.10E-02	0.02%	0.07%	4.73%	0.45%	2.13%	4.50%	81.82%	4.68%	0.11%	0.06%	1.43%
67	4.960	1.10E-02	0.26%	0.07%	19.63%	7.90%	3.93%	39.36%	21.70%	1.05%	1.80%	0.11%	4.21%
68	4.971	5.20E-02	0.26%	0.04%	12.85%	11.20%	0.41%	47.55%	13.81%	0.50%	6.61%	0.01%	6.75%
69	4.987	6.00E-03	0.14%	0.03%	6.34%	5.17%	1.96%	16.23%	64.95%	1.82%	1.15%	0.04%	2.17%
70	4.997	2.30E-02	0.90%	0.01%	7.01%	36.47%	0.15%	36.49%	0.72%	0.04%	10.85%	0.00%	7.36%
71	5.007	2.10E-02	0.73%	0.02%	13.67%	37.32%	0.91%	11.92%	16.86%	0.64%	10.82%	0.03%	7.09%
72	5.020	2.00E-03	0.03%	0.00%	7.99%	0.86%	1.03%	3.33%	82.28%	3.91%	0.12%	0.05%	0.40%
73	5.026	1.50E-02	0.05%	0.01%	34.57%	1.97%	0.66%	15.38%	43.67%	1.93%	0.22%	0.02%	1.53%
74	5.035	1.00E-02	0.03%	0.01%	31.61%	1.56%	0.64%	8.56%	54.31%	2.21%	0.13%	0.02%	0.93%
75	5.038	1.40E-02	0.25%	0.01%	31.15%	7.19%	0.52%	52.78%	3.26%	0.13%	0.89%	0.02%	3.83%
76	5.080	7.10E-02	0.02%	0.01%	86.72%	2.40%	0.26%	7.04%	1.86%	0.07%	0.05%	0.01%	1.57%
77	5.088	1.00E-03	0.05%	0.06%	14.99%	1.61%	2.25%	9.38%	66.25%	3.05%	0.26%	0.05%	2.06%
78	5.108	1.70E-02	0.08%	0.03%	17.33%	2.90%	2.16%	52.61%	19.77%	1.05%	0.31%	0.08%	3.68%
79	5.130	8.00E-03	0.02%	0.02%	4.56%	0.25%	0.96%	2.39%	86.97%	3.38%	0.67%	0.03%	0.76%
80	5.136	5.00E-03	0.02%	0.03%	4.01%	0.31%	0.93%	4.29%	86.69%	2.64%	0.48%	0.02%	0.60%