Photophysical and Photochemical Studies of Tricarbonyl Rhenium(I) N-Heterocyclic Carbene Complexes Containing Azide and Triazolate Ligands

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Electronic Supplementary Information

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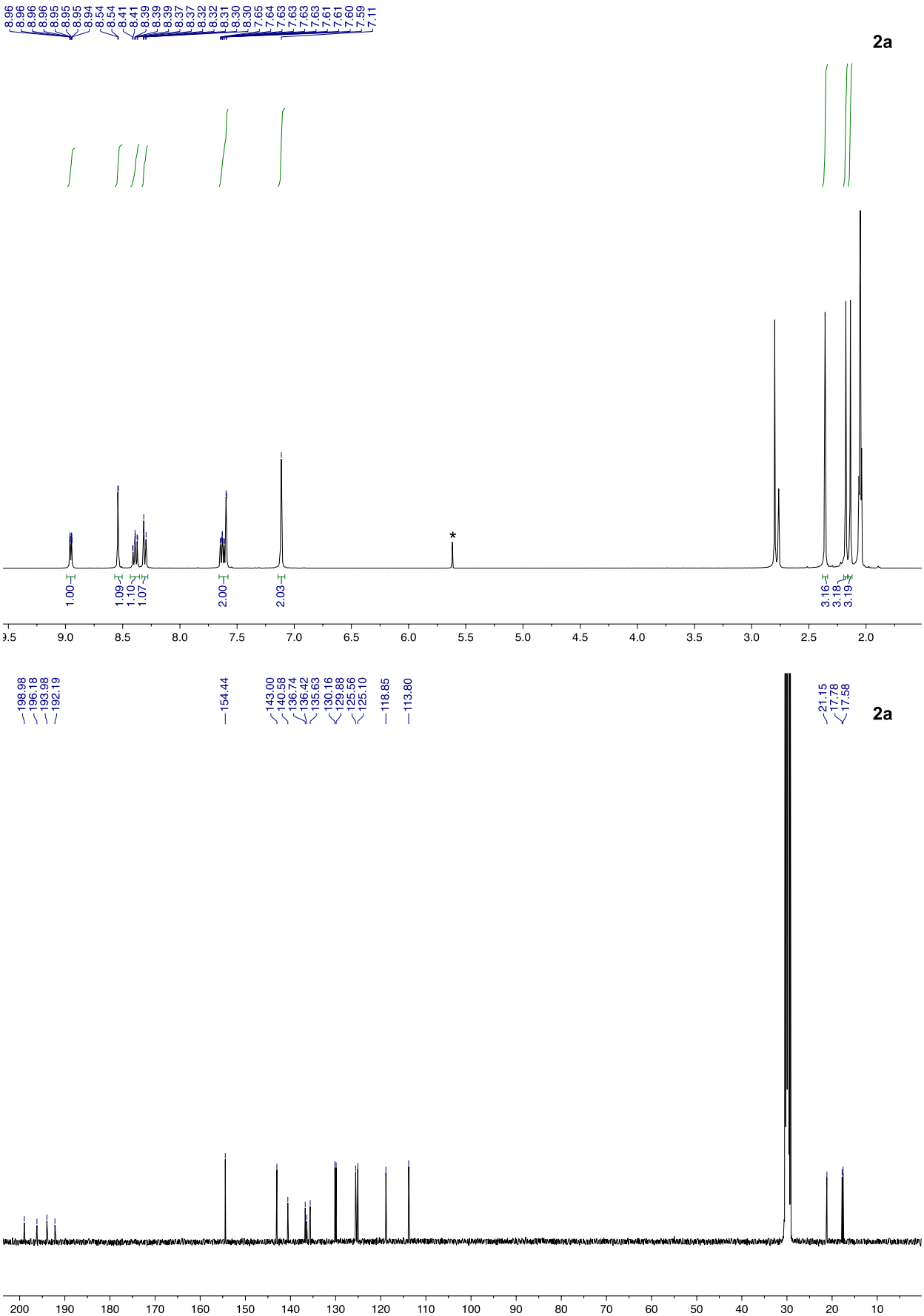

Figure S1. ^{1}H and ^{13}C NMR spectra of a d_6-acetone solution of **2a**.

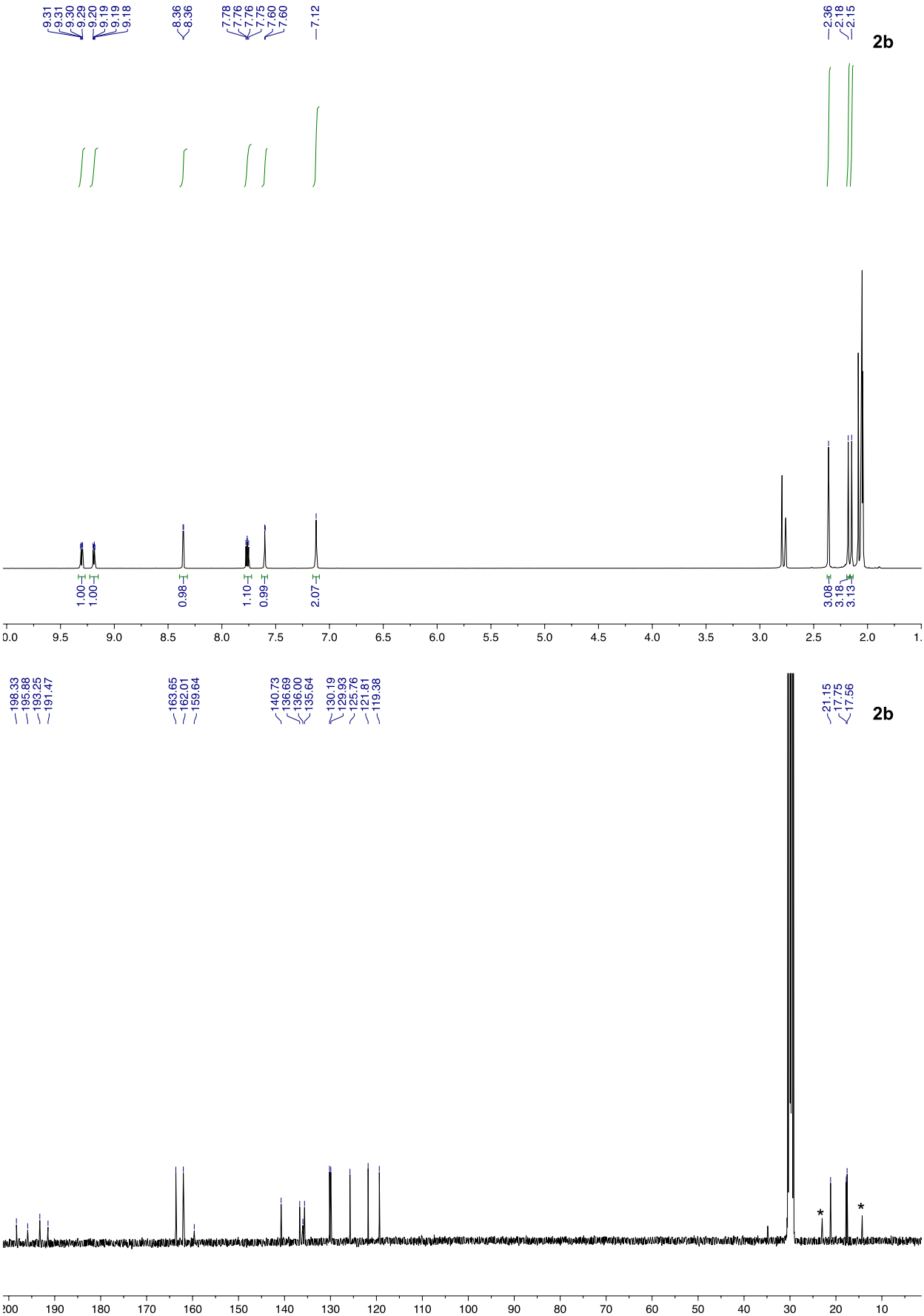

Figure S2. ^{1}H and ^{13}C NMR spectra of a d_6-acetone solution of **2b**.

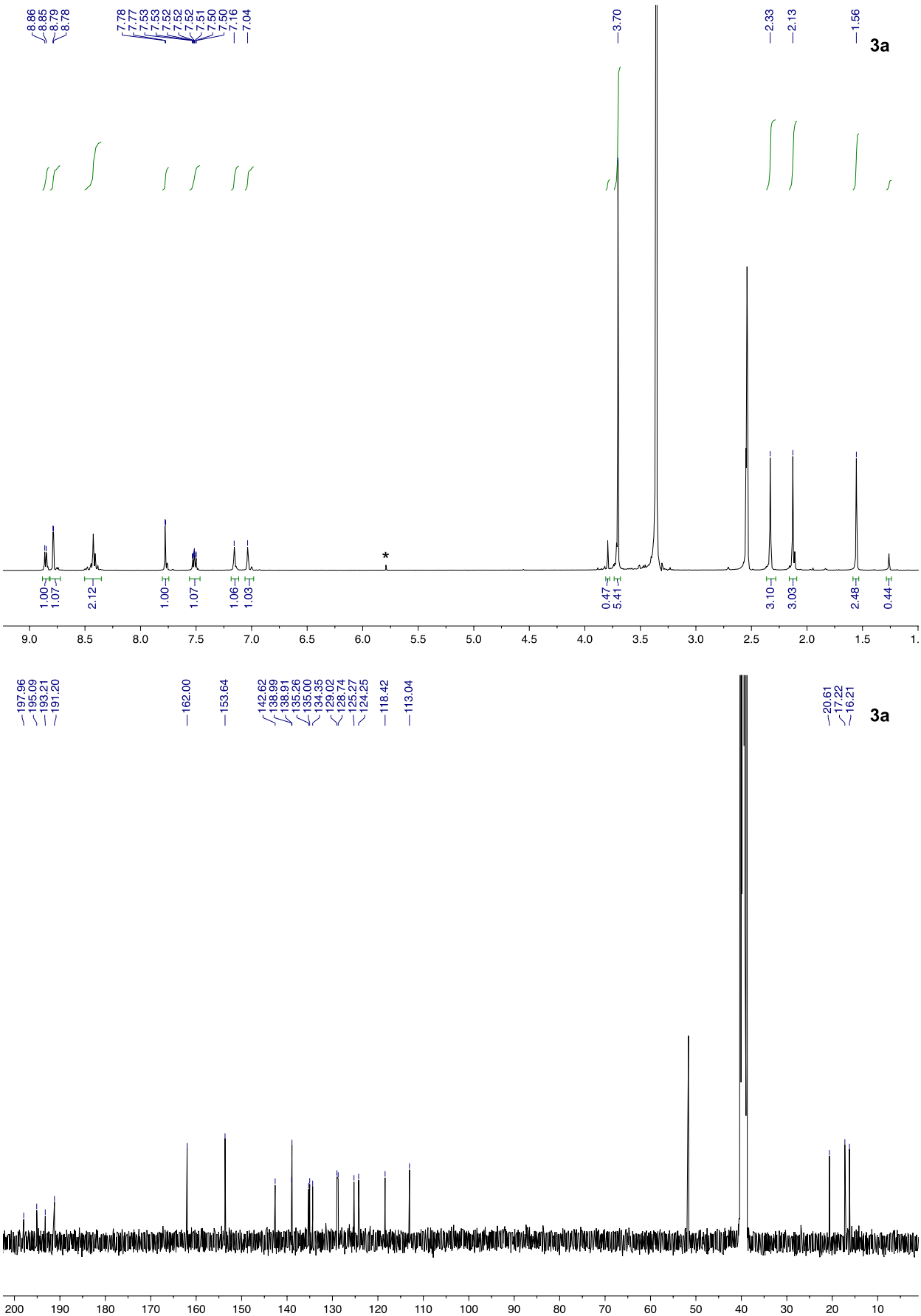

Figure S3. ^{1}H and ^{13}C NMR spectra of a d_6-DMSO solution of **3a**.

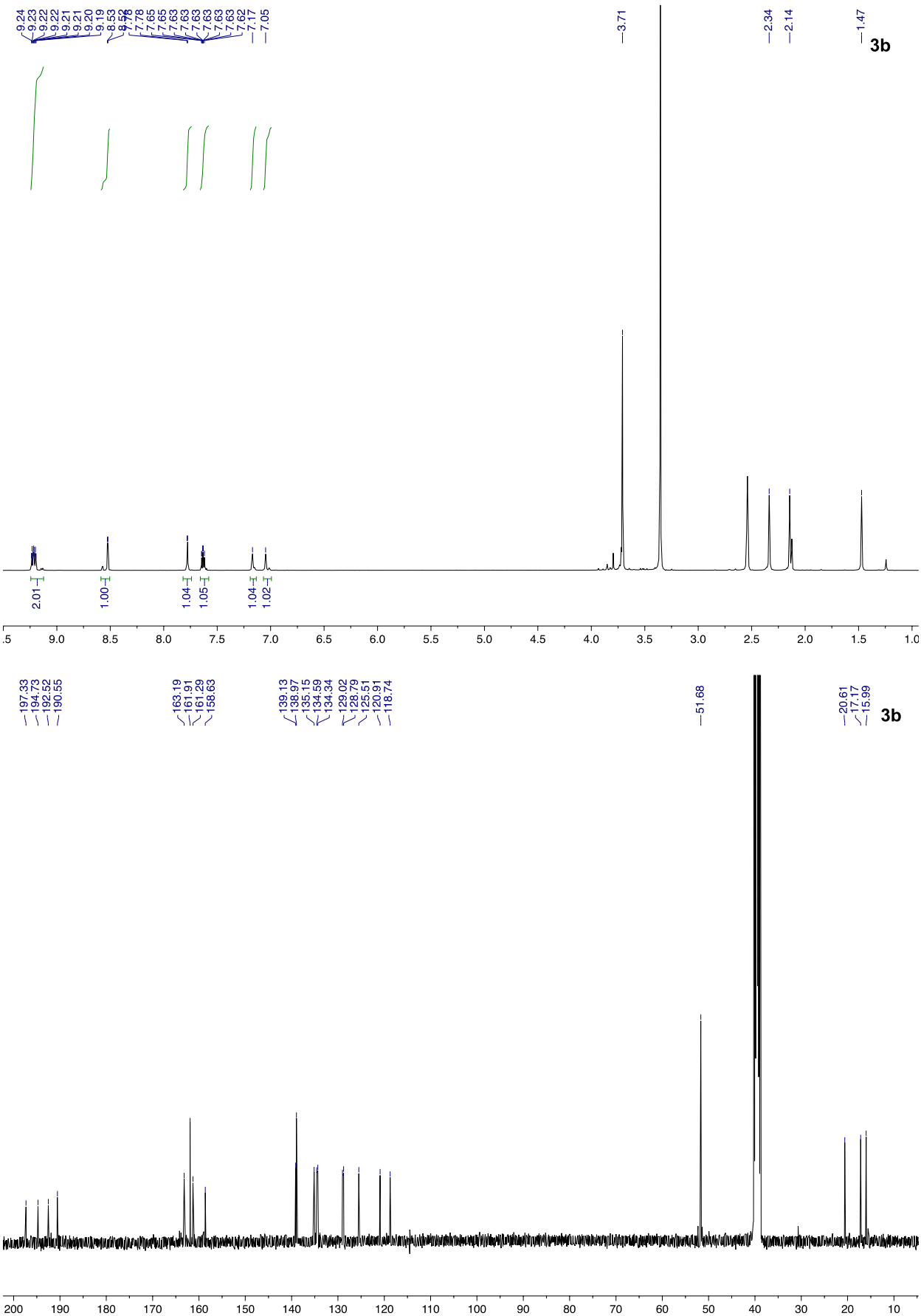

Figure S4. ^{1}H and ^{13}C NMR spectra of a d_6-DMSO solution of **3b**.

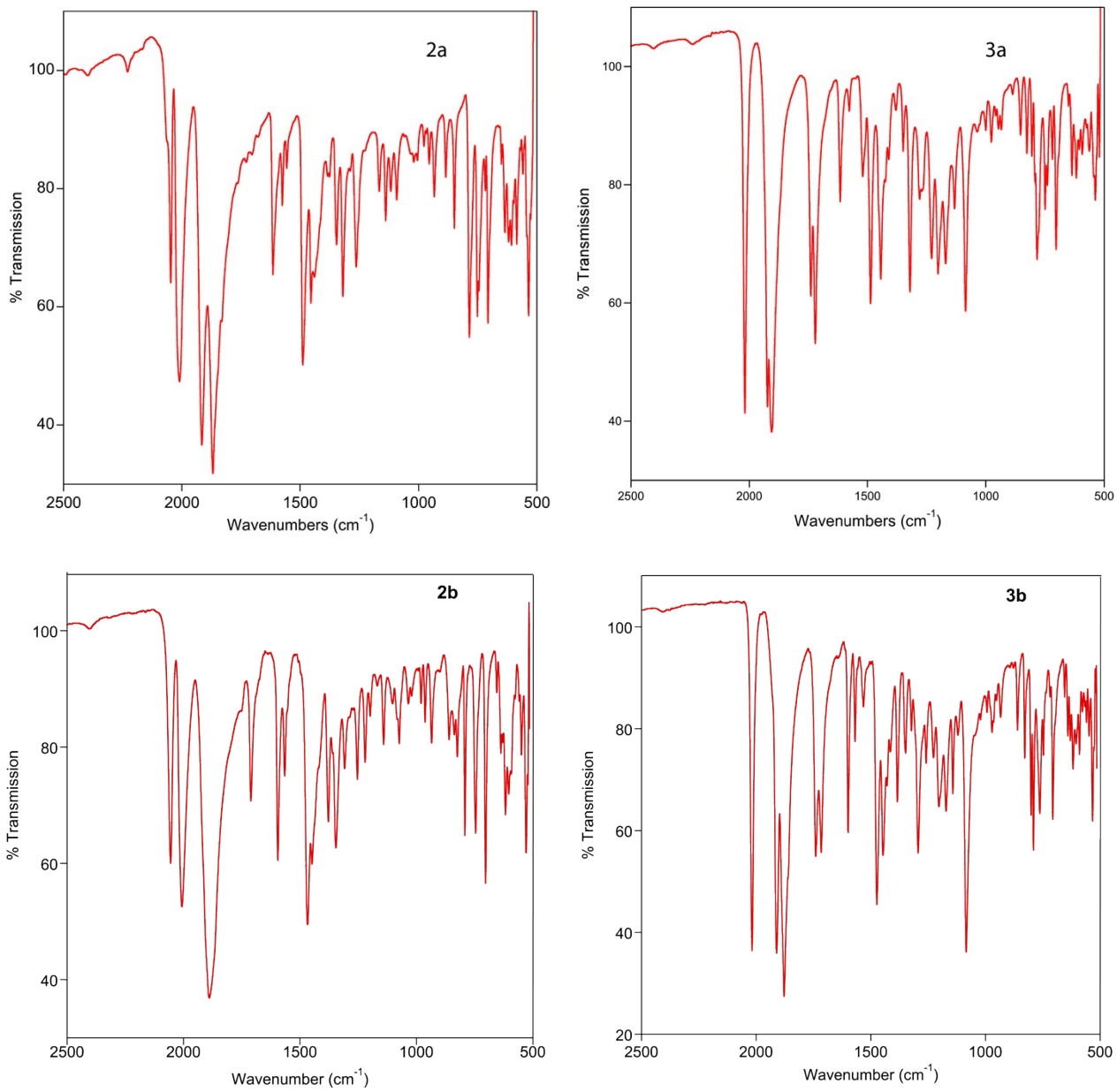

Figure S5. IR spectra of complexes **2a**,**b** and **3a**,**b**.

Table S1. Selected bond lengths [Å] and angles [°] for **2a**.

Re(1)-C(101)	1.906(4)
Re(1)-C(103)	1.913(4)
Re(1)-C(102)	1.965(4)
Re(1)-C(2)	2.122(4)
Re(1)-N(21)	2.202(3)
Re(1)-N(31)	2.202(4)
C(101)-Re(1)-C(103)	88.60(17)
C(101)-Re(1)-C(102)	90.36(16)
C(103)-Re(1)-C(102)	89.20(17)
C(101)-Re(1)-C(2)	91.02(15)
C(103)-Re(1)-C(2)	98.22(16)
C(102)-Re(1)-C(2)	172.48(14)
C(101)-Re(1)-N(21)	94.66(13)
C(103)-Re(1)-N(21)	171.45(14)
C(102)-Re(1)-N(21)	98.66(14)
C(2)-Re(1)-N(21)	73.86(13)
C(101)-Re(1)-N(31)	176.07(13)
C(103)-Re(1)-N(31)	94.84(15)
C(102)-Re(1)-N(31)	91.57(15)
C(2)-Re(1)-N(31)	86.63(14)
N(21)-Re(1)-N(31)	81.67(12)

Table S2. Selected bond lengths [Å] and angles [°] for **2b**.

Re(1)-C(103)	1.926(5)
Re(1)-C(102)	1.930(5)
Re(1)-C(101)	1.963(5)
Re(1)-C(2)	2.118(5)
Re(1)-N(21)	2.194(4)
Re(1)-N(11)	2.196(4)
C(103)-Re(1)-C(102)	90.8(2)
C(103)-Re(1)-C(101)	89.0(2)
C(102)-Re(1)-C(101)	89.5(2)
C(103)-Re(1)-C(2)	92.1(2)
C(102)-Re(1)-C(2)	98.2(2)
C(101)-Re(1)-C(2)	172.2(2)
C(103)-Re(1)-N(21)	93.72(19)
C(102)-Re(1)-N(21)	171.49(18)
C(101)-Re(1)-N(21)	97.80(19)
C(2)-Re(1)-N(21)	74.44(18)
C(103)-Re(1)-N(11)	175.88(19)
C(102)-Re(1)-N(11)	91.8(2)
C(101)-Re(1)-N(11)	94.24(19)
C(2)-Re(1)-N(11)	84.37(18)
N(21)-Re(1)-N(11)	83.30(16)

Table S3. Selected bond lengths [Å] and angles [°] for **3a**.

Re(1)-C(101)	1.922(3)
Re(1)-C(103)	1.930(3)
Re(1)-C(102)	1.949(3)
Re(1)-C(2)	2.125(3)
Re(1)-N(42)	2.172(2)
Re(1)-N(21)	2.197(2)
C(101)-Re(1)-C(103)	88.94(13)
C(101)-Re(1)-C(102)	89.65(12)
C(103)-Re(1)-C(102)	90.74(13)
C(101)-Re(1)-C(2)	94.58(11)
C(103)-Re(1)-C(2)	99.24(12)
C(102)-Re(1)-C(2)	169.22(11)
C(101)-Re(1)-N(42)	178.10(11)
C(103)-Re(1)-N(42)	89.17(11)
C(102)-Re(1)-N(42)	90.49(11)
C(2)-Re(1)-N(42)	85.61(10)
C(101)-Re(1)-N(21)	94.46(11)
C(103)-Re(1)-N(21)	172.82(11)
C(102)-Re(1)-N(21)	95.60(10)
C(2)-Re(1)-N(21)	74.22(10)
N(42)-Re(1)-N(21)	87.41(9)

Table S4. Selected bond lengths [Å] and angles [°] for **3b**.

Re(1)-C(101)	1.920(2)
Re(1)-C(103)	1.926(2)
Re(1)-C(102)	1.949(2)
Re(1)-C(2)	2.134(2)
Re(1)-N(42)	2.1657(18)
Re(1)-N(21)	2.2100(18)
C(101)-Re(1)-C(103)	89.38(10)
C(101)-Re(1)-C(102)	90.88(10)
C(103)-Re(1)-C(102)	90.96(9)
C(101)-Re(1)-C(2)	92.20(10)
C(103)-Re(1)-C(2)	97.74(9)
C(102)-Re(1)-C(2)	170.80(9)
C(101)-Re(1)-N(42)	178.12(9)
C(103)-Re(1)-N(42)	88.79(8)
C(102)-Re(1)-N(42)	89.55(8)
C(2)-Re(1)-N(42)	87.64(7)
C(101)-Re(1)-N(21)	95.22(8)
C(103)-Re(1)-N(21)	170.94(8)
C(102)-Re(1)-N(21)	96.76(8)
C(2)-Re(1)-N(21)	74.33(8)
N(42)-Re(1)-N(21)	86.54(7)

Figure S6. Excitation spectra of all complexes from a *ca* 10^{-5} M solution in dichloromethane.

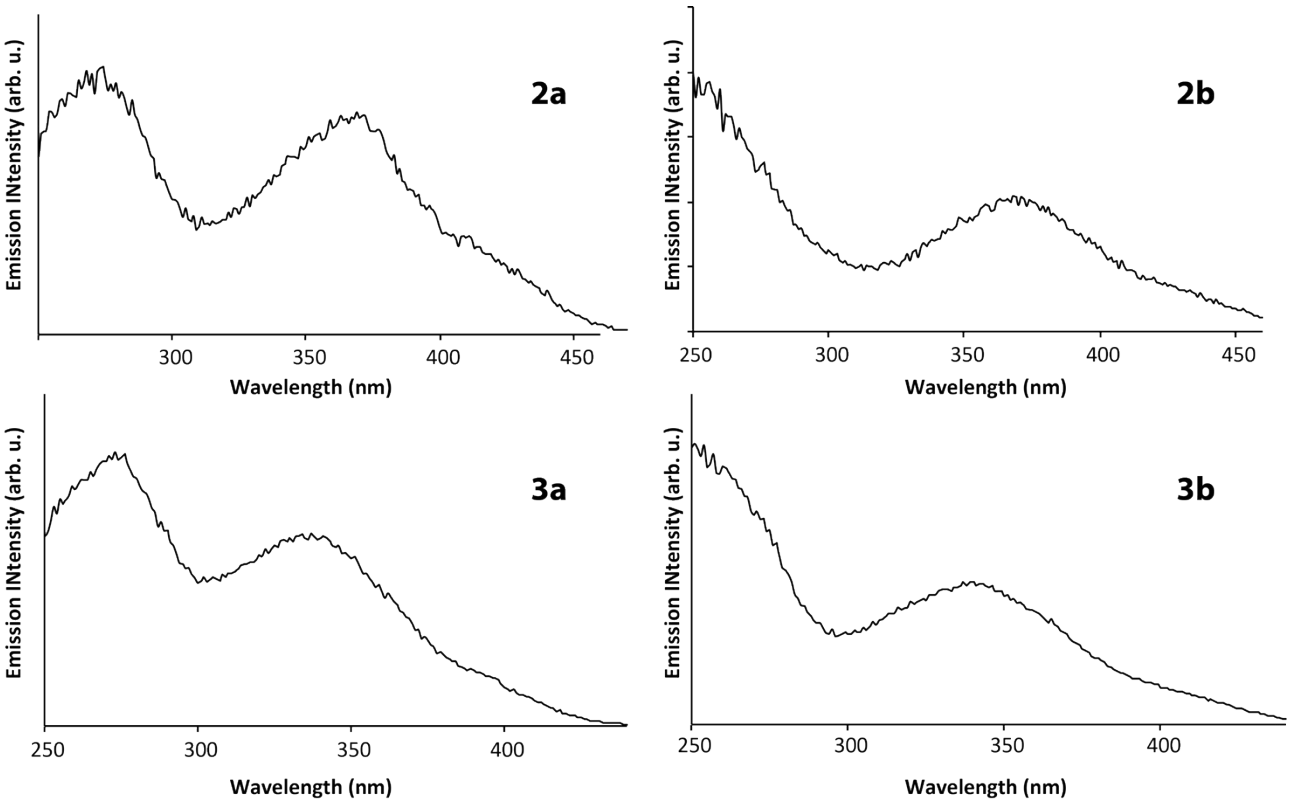

Figure S7. Excitation and emission spectra of all complexes from a *ca* 10^{-5} M solution in dichloromethane at 77 K.

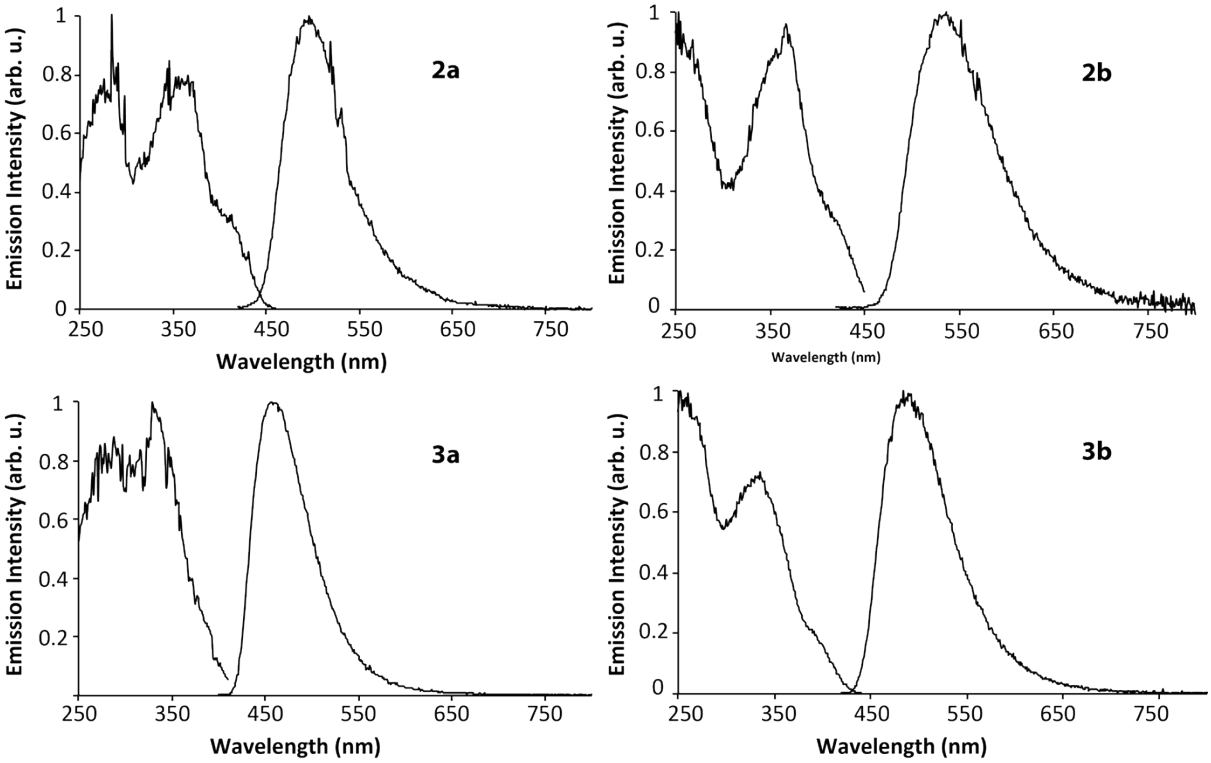

Figure S8. Selected occupied orbital contours of **3a**, **2b**, and **3b**.

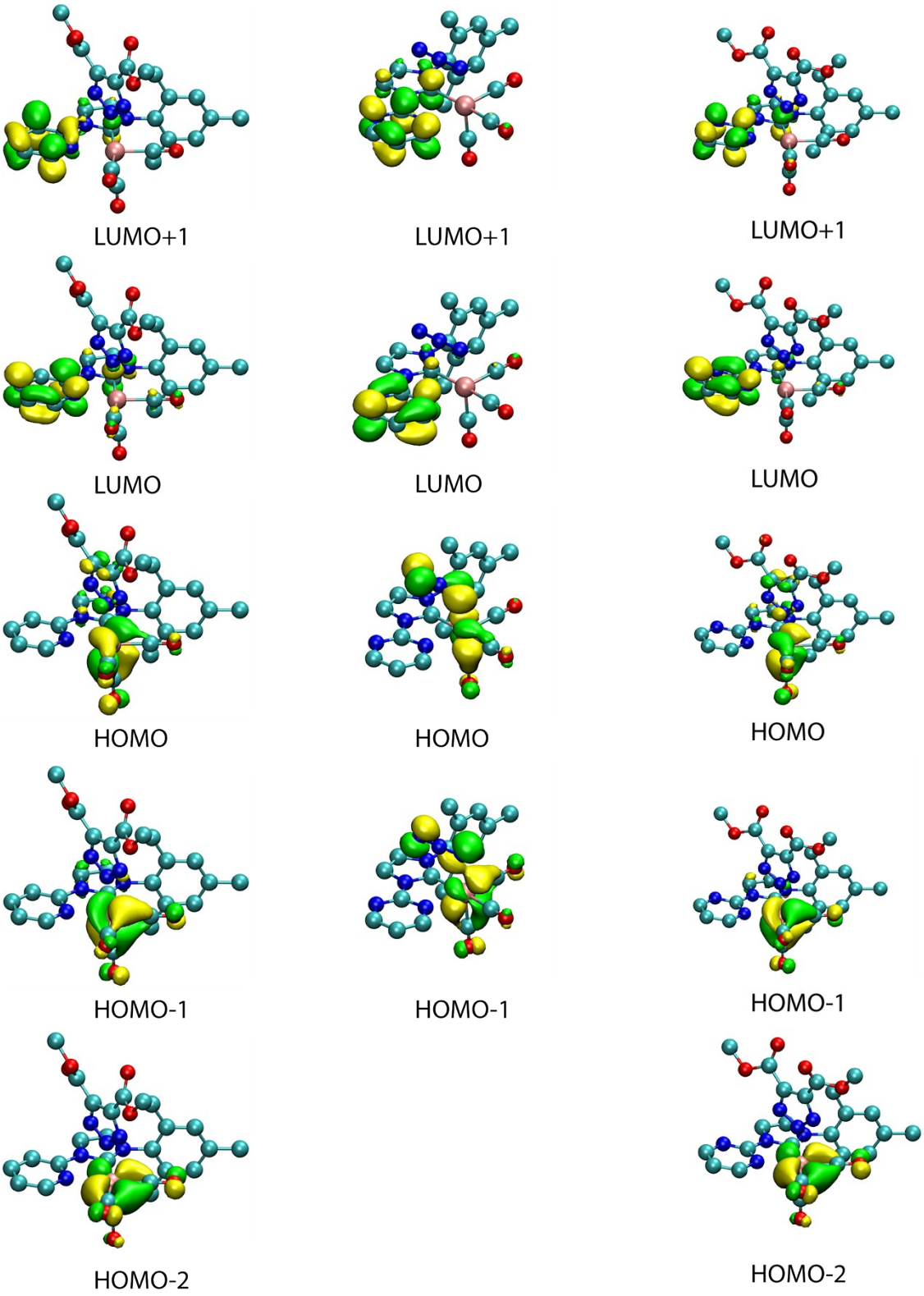

Table S5. Calculated transitions for **2a**.

Wavelength	**Intensity**	**Levels**	**Character**
468.04 nm	0.0054	HOMO -> LUMO	99.10%
390.33 nm	0.0674	HOMO-1 -> LUMO	95.50%
		HOMO -> LUMO+1	3.10%
378.34 nm	0.0203	HOMO-1 -> LUMO	3.20%
		HOMO -> LUMO+1	95.70%
351.85 nm	0.0006	HOMO-2 -> LUMO	95.60%
332.21 nm	0.0344	HOMO-3 -> LUMO	12.00%
		HOMO -> LUMO+2	79.30%
331.33 nm	0.0099	HOMO-3 -> LUMO	7.10%
		HOMO-1 -> LUMO+1	90.80%
327.62 nm	0.0377	HOMO-3 -> LUMO	76.00%
		HOMO-1 -> LUMO+1	6.50%
		HOMO -> LUMO+2	11.80%
315.72 nm	0.0273	HOMO-6 -> LUMO	5.10%
		HOMO-5 -> LUMO	3.80%
		HOMO-4 -> LUMO	4.70%
		HOMO-2 -> LUMO+2	2.80%
		HOMO-1 -> LUMO+2	5.70%
		HOMO -> LUMO+3	67.70%
		HOMO -> LUMO+4	2.40%
310.81 nm	0.0762	HOMO-6 -> LUMO	27.60%
		HOMO-5 -> LUMO	21.90%
		HOMO-4 -> LUMO	30.10%
		HOMO-3 -> LUMO	2.50%
		HOMO -> LUMO+3	12.60%

301.97 nm	0.0149	HOMO-1 -> LUMO+2	75.00%
		HOMO-1 -> LUMO+3	7.00%
		HOMO-1 -> LUMO+4	3.40%
		HOMO -> LUMO+3	7.40%
295.09 nm	0.001	HOMO-2 -> LUMO+1	94.40%
		HOMO-2 -> LUMO+3	2.50%
294.42 nm	0.003	HOMO-6 -> LUMO	18.40%
		HOMO-5 -> LUMO	17.80%
		HOMO-4 -> LUMO	62.20%
293.28 nm	0.0024	HOMO-6 -> LUMO	43.90%
		HOMO-5 -> LUMO	52.90%
284.74 nm	0.0016	HOMO-3 -> LUMO+1	5.90%
		HOMO-1 -> LUMO+3	2.50%
		HOMO -> LUMO+2	2.40%
		HOMO -> LUMO+3	2.60%
		HOMO -> LUMO+4	80.40%
		HOMO -> LUMO+7	2.80%
283.31 nm	0.0469	HOMO-3 -> LUMO+1	80.50%
		HOMO-2 -> LUMO+2	2.10%
		HOMO-1 -> LUMO+3	4.10%
		HOMO -> LUMO+4	8.90%
281.18 nm	0.0069	HOMO-3 -> LUMO+1	7.00%
		HOMO-1 -> LUMO+2	7.10%
		HOMO-1 -> LUMO+3	69.50%
		HOMO -> LUMO+9	3.10%
275.37 nm	0.0007	HOMO-7 -> LUMO	5.80%
		HOMO-6 -> LUMO+1	7.80%
		HOMO-5 -> LUMO+1	5.60%
		HOMO-4 -> LUMO+1	6.40%

		HOMO-3 -> LUMO+1	2.80%
		HOMO-2 -> LUMO+2	3.90%
		HOMO -> LUMO+5	7.00%
		HOMO -> LUMO+7	18.90%
		HOMO -> LUMO+9	2.20%
		HOMO -> LUMO+10	11.50%
		HOMO -> LUMO+11	5.00%
		HOMO -> LUMO+13	2.20%
		HOMO -> LUMO+14	2.10%
		HOMO -> LUMO+15	5.10%
272.36 nm	0.0173	HOMO-7 -> LUMO	8.80%
		HOMO-6 -> LUMO+1	17.40%
		HOMO-5 -> LUMO+1	12.60%
		HOMO-4 -> LUMO+1	15.10%
		HOMO -> LUMO+5	35.20%
		HOMO -> LUMO+10	2.70%
271.57 nm	0.0228	HOMO-6 -> LUMO+1	5.00%
		HOMO-5 -> LUMO+1	3.80%
		HOMO-4 -> LUMO+1	4.60%
		HOMO -> LUMO+5	51.10%
		HOMO -> LUMO+7	20.90%
		HOMO -> LUMO+10	2.60%
268.99 nm	0.0066	HOMO-2 -> LUMO+2	52.50%
		HOMO-2 -> LUMO+3	6.90%
		HOMO-2 -> LUMO+7	2.20%
		HOMO-1 -> LUMO+7	2.90%
		HOMO -> LUMO+6	2.20%
		HOMO -> LUMO+7	9.70%
		HOMO -> LUMO+9	3.90%
267.10 nm	0.0198	HOMO-7 -> LUMO	3.30%
		HOMO-2 -> LUMO+2	6.80%
		HOMO-2 -> LUMO+3	5.20%
		HOMO -> LUMO+3	3.10%

		HOMO -> LUMO+5	4.30%
		HOMO -> LUMO+6	13.00%
		HOMO -> LUMO+7	19.20%
		HOMO -> LUMO+9	14.50%
		HOMO -> LUMO+10	7.00%
		HOMO -> LUMO+12	2.40%
		HOMO -> LUMO+15	3.90%
262.36 nm	0.0144	HOMO-7 -> LUMO	9.40%
		HOMO-4 -> LUMO+1	2.00%
		HOMO-2 -> LUMO+3	43.90%
		HOMO-2 -> LUMO+4	2.60%
		HOMO-1 -> LUMO+4	3.70%
		HOMO-1 -> LUMO+7	4.10%
		HOMO -> LUMO+6	2.50%
		HOMO -> LUMO+8	4.20%
		HOMO -> LUMO+9	6.40%
		HOMO -> LUMO+10	5.10%
261.31 nm	0.1332	HOMO-7 -> LUMO	36.80%
		HOMO-4 -> LUMO+1	6.10%
		HOMO-2 -> LUMO+3	2.30%
		HOMO-1 -> LUMO+4	2.60%
		HOMO-1 -> LUMO+7	2.90%
		HOMO -> LUMO+6	5.80%
		HOMO -> LUMO+8	8.10%
		HOMO -> LUMO+9	11.10%
		HOMO -> LUMO+10	2.80%
		HOMO -> LUMO+12	2.70%
259.09 nm	0.1536	HOMO-7 -> LUMO	22.20%
		HOMO-4 -> LUMO+1	9.60%
		HOMO-3 -> LUMO+3	3.70%
		HOMO-2 -> LUMO+2	4.50%
		HOMO-2 -> LUMO+3	18.20%
		HOMO-1 -> LUMO+9	3.30%
		HOMO -> LUMO+8	6.30%

		HOMO -> LUMO+9	11.50%
257.62 nm	0.0116	HOMO-3 -> LUMO+2	3.20%
		HOMO-2 -> LUMO+3	2.80%
		HOMO-1 -> LUMO+2	2.00%
		HOMO-1 -> LUMO+3	3.30%
		HOMO-1 -> LUMO+4	80.20%

Table S6. Calculated transitions for **2b**.

Wavelength	Intensity	Levels	Character
502.79 nm	0.004	HOMO -> LUMO	98.10%
439.27 nm	0.0049	HOMO -> LUMO+1	97.00%
411.91 nm	0.0691	HOMO-1 -> LUMO	97.70%
374.15 nm	0.0114	HOMO-1 -> LUMO+1	98.30%
366.50 nm	0.0005	HOMO-2 -> LUMO	93.30%
		HOMO-2 -> LUMO+1	3.60%
343.58 nm	0.0204	HOMO-3 -> LUMO	94.60%
334.01 nm	0.0298	HOMO -> LUMO+2	90.80%
328.78 nm	0.0012	HOMO-2 -> LUMO	3.90%
		HOMO-2 -> LUMO+1	93.00%
324.43 nm	0.0582	HOMO-6 -> LUMO	59.90%
		HOMO-5 -> LUMO	9.60%
		HOMO-4 -> LUMO	15.80%
		HOMO-3 -> LUMO	2.20%
		HOMO-3 -> LUMO+1	4.70%
		HOMO -> LUMO+3	3.30%
318.17 nm	0.0159	HOMO-3 -> LUMO+1	6.10%
		HOMO-1 -> LUMO+2	4.90%
		HOMO -> LUMO+3	77.50%
313.34 nm	0.0833	HOMO-6 -> LUMO	2.50%
		HOMO-4 -> LUMO	5.00%
		HOMO-3 -> LUMO+1	84.90%
		HOMO -> LUMO+3	3.40%

309.57 nm	0.0088	HOMO-6 -> LUMO	13.70%
		HOMO-5 -> LUMO	7.70%
		HOMO-4 -> LUMO	73.20%
		HOMO-4 -> LUMO+1	3.40%
307.62 nm	0.0053	HOMO-6 -> LUMO	17.40%
		HOMO-5 -> LUMO	73.90%
		HOMO-5 -> LUMO+1	5.20%
302.29 nm	0.0179	HOMO-6 -> LUMO+1	2.10%
		HOMO-1 -> LUMO+2	74.00%
		HOMO-1 -> LUMO+3	8.20%
		HOMO -> LUMO+3	6.20%
299.04 nm	0.013	HOMO-6 -> LUMO+1	65.40%
		HOMO-5 -> LUMO+1	10.00%
		HOMO-4 -> LUMO+1	16.50%
		HOMO-1 -> LUMO+2	2.20%
286.79 nm	0.0003	HOMO-6 -> LUMO+1	11.90%
		HOMO-5 -> LUMO+1	5.90%
		HOMO-4 -> LUMO	3.10%
		HOMO-4 -> LUMO+1	77.70%
285.11 nm	0.0003	HOMO-6 -> LUMO+1	14.70%
		HOMO-5 -> LUMO	5.00%
		HOMO-5 -> LUMO+1	76.10%
283.20 nm	0.0116	HOMO-1 -> LUMO+2	6.50%
		HOMO-1 -> LUMO+3	62.10%
		HOMO -> LUMO+4	18.30%
		HOMO -> LUMO+7	2.20%
282.12 nm	0.0103	HOMO-1 -> LUMO+2	2.80%
		HOMO-1 -> LUMO+3	16.10%
		HOMO -> LUMO+4	70.60%

		HOMO -> LUMO+7	2.60%
274.53 nm	0.0099	HOMO-2 -> LUMO+2	7.90%
		HOMO -> LUMO+4	5.70%
		HOMO -> LUMO+5	5.00%
		HOMO -> LUMO+7	30.30%
		HOMO -> LUMO+10	18.20%
		HOMO -> LUMO+12	3.70%
		HOMO -> LUMO+14	5.50%
		HOMO -> LUMO+15	3.50%
270.64 nm	0.0076	HOMO-2 -> LUMO+2	55.30%
		HOMO-2 -> LUMO+3	13.20%
		HOMO-2 -> LUMO+7	2.10%
		HOMO -> LUMO+6	2.50%
		HOMO -> LUMO+7	10.20%
269.46 nm	0.0088	HOMO -> LUMO+5	77.60%
		HOMO -> LUMO+6	5.00%
		HOMO -> LUMO+7	9.30%
266.77 nm	0.0122	HOMO-2 -> LUMO+3	6.80%
		HOMO -> LUMO+5	16.60%
		HOMO -> LUMO+6	19.00%
		HOMO -> LUMO+7	11.90%
		HOMO -> LUMO+8	9.20%
		HOMO -> LUMO+9	3.30%
		HOMO -> LUMO+10	8.80%
		HOMO -> LUMO+12	4.20%
		HOMO -> LUMO+14	2.60%
		HOMO -> LUMO+15	2.40%
264.56 nm	0.0141	HOMO-7 -> LUMO	76.80%
		HOMO-2 -> LUMO+3	16.50%
262.03 nm	0.0319	HOMO-7 -> LUMO	9.40%
		HOMO-2 -> LUMO+2	2.90%

		HOMO-2 -> LUMO+3	25.30%
		HOMO-1 -> LUMO+4	2.80%
		HOMO-1 -> LUMO+7	6.10%
		HOMO -> LUMO+6	7.00%
		HOMO -> LUMO+8	16.50%
		HOMO -> LUMO+10	6.80%
		HOMO -> LUMO+12	4.00%

Table S7. Calculated transitions for **3a**.

Wavelength	Intensity	Levels	Character
388.42 nm	0.0099	HOMO -> LUMO	98.20%
352.03 nm	0.0454	HOMO-2 -> LUMO	36.80%
		HOMO-1 -> LUMO	59.50%
341.57 nm	0.1226	HOMO-2 -> LUMO	59.20%
		HOMO-1 -> LUMO	35.90%
		HOMO -> LUMO+1	2.10%
322.23 nm	0.0606	HOMO-1 -> LUMO	2.30%
		HOMO -> LUMO+1	94.60%
305.23 nm	0.0672	HOMO -> LUMO+2	7.70%
		HOMO -> LUMO+3	80.10%
		HOMO -> LUMO+7	3.10%
299.62 nm	0.0065	HOMO-1 -> LUMO+1	93.30%
293.28 nm	0.0005	HOMO-4 -> LUMO	6.70%
		HOMO-3 -> LUMO	91.70%
292.39 nm	0.0373	HOMO-4 -> LUMO	4.60%
		HOMO-1 -> LUMO+3	4.00%
		HOMO -> LUMO+2	78.90%
		HOMO -> LUMO+3	6.70%
		HOMO -> LUMO+4	2.10%
292.10 nm	0.0044	HOMO-4 -> LUMO	84.80%
		HOMO-3 -> LUMO	6.60%
		HOMO -> LUMO+2	5.00%
290.90 nm	0.0019	HOMO-2 -> LUMO+1	92.50%

290.32 nm	0.01	HOMO-1 -> LUMO+2	5.80%
		HOMO-1 -> LUMO+3	64.40%
		HOMO-1 -> LUMO+7	2.50%
		HOMO -> LUMO+2	6.70%
		HOMO -> LUMO+4	11.00%
280.96 nm	0.0364	HOMO-2 -> LUMO+3	22.30%
		HOMO-1 -> LUMO+3	10.30%
		HOMO-1 -> LUMO+4	2.10%
		HOMO -> LUMO+4	42.20%
		HOMO -> LUMO+5	3.40%
		HOMO -> LUMO+9	4.00%
277.93 nm	0.0438	HOMO-5 -> LUMO	91.70%
		HOMO-2 -> LUMO+3	2.60%
272.35 nm	0.0034	HOMO-2 -> LUMO+2	2.90%
		HOMO-2 -> LUMO+3	5.50%
		HOMO-1 -> LUMO+2	79.60%
		HOMO-1 -> LUMO+3	5.10%
268.33 nm	0.0292	HOMO-6 -> LUMO	4.60%
		HOMO-2 -> LUMO+1	2.10%
		HOMO-2 -> LUMO+2	7.20%
		HOMO-2 -> LUMO+3	34.30%
		HOMO-2 -> LUMO+4	10.60%
		HOMO-2 -> LUMO+9	2.00%
		HOMO-1 -> LUMO+2	9.20%
		HOMO-1 -> LUMO+3	3.70%
		HOMO -> LUMO+4	13.80%
		HOMO -> LUMO+9	2.60%
264.02 nm	0.0003	HOMO-2 -> LUMO+2	68.70%
		HOMO-2 -> LUMO+3	4.90%
		HOMO-2 -> LUMO+4	10.60%
		HOMO-1 -> LUMO+4	8.20%

262.73 nm	0.0335	HOMO-6 -> LUMO	16.80%
		HOMO-2 -> LUMO+2	14.60%
		HOMO-2 -> LUMO+4	5.50%
		HOMO-1 -> LUMO+4	37.40%
		HOMO-1 -> LUMO+5	4.70%
		HOMO -> LUMO+7	2.10%
260.04 nm	0.1163	HOMO-6 -> LUMO	63.70%
		HOMO-5 -> LUMO+1	3.00%
		HOMO-2 -> LUMO+3	4.00%
		HOMO-1 -> LUMO+4	12.10%
		HOMO -> LUMO+7	2.50%
257.34 nm	0.0364	HOMO-2 -> LUMO+3	2.90%
		HOMO-2 -> LUMO+4	19.70%
		HOMO-2 -> LUMO+5	2.90%
		HOMO -> LUMO+4	6.80%
		HOMO -> LUMO+5	45.10%
		HOMO -> LUMO+7	6.00%
		HOMO -> LUMO+9	5.30%
256.05 nm	0.037	HOMO-7 -> LUMO	67.20%
		HOMO-6 -> LUMO	4.40%
		HOMO-3 -> LUMO+1	13.90%
		HOMO -> LUMO+7	3.90%
255.76 nm	0.0084	HOMO-7 -> LUMO	10.80%
		HOMO-3 -> LUMO+1	83.80%
254.29 nm	0.0112	HOMO-4 -> LUMO+1	74.50%
		HOMO-2 -> LUMO+4	2.50%
		HOMO -> LUMO+5	10.00%
		HOMO -> LUMO+7	2.40%
254.04 nm	0.0395	HOMO-7 -> LUMO	2.30%
		HOMO-4 -> LUMO+1	21.30%
		HOMO-2 -> LUMO+3	2.50%

		HOMO-2 -> LUMO+4	12.00%
		HOMO-2 -> LUMO+5	2.40%
		HOMO -> LUMO+5	29.40%
		HOMO -> LUMO+7	13.30%
		HOMO -> LUMO+9	2.10%
		HOMO -> LUMO+11	2.20%
252.12 nm	0.2242	HOMO-7 -> LUMO	4.10%
		HOMO-2 -> LUMO+4	9.90%
		HOMO-1 -> LUMO+4	9.40%
		HOMO -> LUMO+3	3.10%
		HOMO -> LUMO+5	2.00%
		HOMO -> LUMO+7	53.70%
		HOMO -> LUMO+9	4.90%
248.37 nm	0.0114	HOMO-10 -> LUMO	2.20%
		HOMO-9 -> LUMO	3.00%
		HOMO-8 -> LUMO	83.30%
		HOMO-5 -> LUMO+1	5.30%

Table S8. Calculated transitions for **3b**.

Wavelength	**Intensity**	**Levels**	**Character**
410.32 nm	0.0098	HOMO -> LUMO	97.20%
368.27 nm	0.0075	HOMO-2 -> LUMO	9.20%
		HOMO-1 -> LUMO	40.70%
		HOMO -> LUMO+1	46.30%
363.85 nm	0.0234	HOMO-2 -> LUMO	38.20%
		HOMO-1 -> LUMO	14.80%
		HOMO -> LUMO+1	42.50%
353.08 nm	0.1606	HOMO-2 -> LUMO	46.80%
		HOMO-1 -> LUMO	42.10%
		HOMO -> LUMO+1	8.30%
332.59 nm	0.0216	HOMO-1 -> LUMO+1	95.80%
323.23 nm	0.0044	HOMO-2 -> LUMO	3.40%
		HOMO-2 -> LUMO+1	92.90%
307.74 nm	0.0005	HOMO-3 -> LUMO	95.20%
		HOMO-3 -> LUMO+1	3.60%
305.86 nm	0.0012	HOMO-4 -> LUMO	88.50%
		HOMO-4 -> LUMO+1	5.30%
		HOMO -> LUMO+3	3.30%
305.33 nm	0.0602	HOMO-4 -> LUMO	3.60%
		HOMO -> LUMO+3	84.70%
		HOMO -> LUMO+7	3.30%
292.55 nm	0.0268	HOMO-5 -> LUMO	2.20%
		HOMO-1 -> LUMO+3	18.10%
		HOMO -> LUMO+2	62.10%

		HOMO -> LUMO+4	11.70%
289.98 nm	0.001	HOMO-5 -> LUMO	86.90%
		HOMO -> LUMO+2	8.20%
288.21 nm	0.0296	HOMO-5 -> LUMO	8.20%
		HOMO-1 -> LUMO+3	46.60%
		HOMO -> LUMO+2	25.50%
		HOMO -> LUMO+4	11.20%
284.66 nm	0.0001	HOMO-3 -> LUMO	3.70%
		HOMO-3 -> LUMO+1	95.00%
283.06 nm	0.0002	HOMO-4 -> LUMO	5.80%
		HOMO-4 -> LUMO+1	91.80%
280.39 nm	0.0494	HOMO-2 -> LUMO+3	23.30%
		HOMO-1 -> LUMO+3	17.30%
		HOMO-1 -> LUMO+4	2.90%
		HOMO -> LUMO+4	39.90%
		HOMO -> LUMO+9	3.70%
270.30 nm	0.0075	HOMO-6 -> LUMO	2.40%
		HOMO-2 -> LUMO+3	11.50%
		HOMO-1 -> LUMO+2	69.50%
		HOMO-1 -> LUMO+4	4.80%
		HOMO -> LUMO+4	2.70%
268.92 nm	0.0335	HOMO-5 -> LUMO+1	9.60%
		HOMO-2 -> LUMO+3	33.90%
		HOMO-2 -> LUMO+4	20.90%
		HOMO-1 -> LUMO+2	7.10%
		HOMO-1 -> LUMO+3	3.30%
		HOMO-1 -> LUMO+4	2.60%
		HOMO -> LUMO+4	9.10%
268.29 nm	0.0597	HOMO-6 -> LUMO	9.20%

		HOMO-5 -> LUMO+1	76.90%
		HOMO-1 -> LUMO+2	5.50%
264.96 nm	0.0241	HOMO-13 -> LUMO	3.50%
		HOMO-12 -> LUMO	2.00%
		HOMO-7 -> LUMO	26.20%
		HOMO-6 -> LUMO	42.20%
		HOMO-5 -> LUMO+1	5.70%
		HOMO-2 -> LUMO+2	3.20%
		HOMO-2 -> LUMO+4	4.20%
		HOMO-1 -> LUMO+2	2.30%
		HOMO-1 -> LUMO+4	4.30%
262.93 nm	0.0085	HOMO-7 -> LUMO	26.10%
		HOMO-2 -> LUMO+2	34.00%
		HOMO-2 -> LUMO+3	2.90%
		HOMO-2 -> LUMO+4	4.80%
		HOMO-1 -> LUMO+2	7.50%
		HOMO-1 -> LUMO+4	14.10%
261.53 nm	0.03	HOMO-9 -> LUMO	2.70%
		HOMO-7 -> LUMO	33.80%
		HOMO-6 -> LUMO	19.20%
		HOMO-5 -> LUMO+1	2.20%
		HOMO-2 -> LUMO+2	31.60%
		HOMO-1 -> LUMO+4	2.50%
260.71 nm	0.0049	HOMO-7 -> LUMO	7.60%
		HOMO-6 -> LUMO	11.50%
		HOMO-2 -> LUMO+2	16.70%
		HOMO-2 -> LUMO+3	2.20%
		HOMO-1 -> LUMO+2	3.40%
		HOMO-1 -> LUMO+4	38.80%
		HOMO -> LUMO+7	5.00%
257.28 nm	0.0016	HOMO-13 -> LUMO	24.10%
		HOMO-12 -> LUMO	30.00%

		HOMO-10 -> LUMO	2.80%
		HOMO-8 -> LUMO	34.60%
255.72 nm	0.0154	HOMO-13 -> LUMO	6.60%
		HOMO-12 -> LUMO	7.00%
		HOMO-8 -> LUMO	24.20%
		HOMO-6 -> LUMO	3.70%
		HOMO-2 -> LUMO+2	4.60%
		HOMO-2 -> LUMO+3	2.80%
		HOMO-2 -> LUMO+4	15.80%
		HOMO -> LUMO+5	15.20%
		HOMO -> LUMO+9	6.00%
255.59 nm	0.0095	HOMO-13 -> LUMO	8.80%
		HOMO-12 -> LUMO	10.40%
		HOMO-10 -> LUMO	2.00%
		HOMO-8 -> LUMO	28.50%
		HOMO-2 -> LUMO+2	3.40%
		HOMO-2 -> LUMO+4	15.20%
		HOMO -> LUMO+5	12.70%
		HOMO -> LUMO+7	2.40%
		HOMO -> LUMO+9	2.90%

Figure S9. Calculated absorption spectra of complexes **2a**, **2b**, **3a**, and **3b**.