Electronic Supplementary Information for Dalton Transactions

ELECTRONIC SUPPLEMENTARY MATERIAL (ESI)

Organometallic red-emitting chromophores: a computational and experimental study on cyclometallated nile red complexes of palladium (II) and platinum(II) acetylacetonates and hexafluoroacetylacetyonates

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Computational Results

In this section, a detailed presentation of the computational results is reported for all the studied compounds. As detailed in the associate paper, all the computations have been performed with the MPW1PW91[1] exchange-correlation functional, the Stuttgart/Dresden ECP basis set[2] on Pd and Pt atoms (SDD keyword of the Gaussian03 suite of programs) and Dunning/Huzinaga valence double-ζ plus polarization D95V(d) basis set[3] on C, N, O, F and H. TD-DFT computations results are listed in the following. They have been performed at the same level of approximation of the previously-performed geometry optimization. The reported computations have been performed in vacuum.

(NR)Pd(acac) (1a)

Table S1. Computed singlet excited states of (NR)Pd(acac) (**1a**). The following text lists the energy (in eV and nm), the oscillator strengths and percentage composition of the most important monoelectronic excitations for each excited state. Excited States composition has been expressed in two ways. The first one uses the Kohn-Sham orbital numerical label of the occupied and virtual orbital as produced by the computation (for instance, 119 -> 120 for the HOMO -> LUMO transition when the HOMO is the 119th orbital and the LUMO is the 120th one). The second way assign the "0" label to the HOMO, the "–1" label to the HOMO-1 orbital and so on, the "0" label to the LUMO, "1" to LUMO+1 and so on (thus, 0 -> 0 is the HOMO -> LUMO transition, -2 -> 1 is the HOMO-2 -> LUMO+1 transition).

Excited State: 1
2.3921 eV 518.31 nm 19293.cm-1 f=0.3690
116 -> 120 4.26 % -3 -> 0
118 -> 120 7.03 % -1 -> 0
119 -> 120 69.47 % 0 -> 0

Excited State: 2
2.7271 eV 454.64 nm 21995.cm-1 f=0.0008
114 -> 120 14.07 % -5 -> 0
117 -> 120 80.33 % -2 -> 0

Excited State: 3
2.8355 eV 437.25 nm 22870.cm-1 f=0.1365
118 -> 120 83.52 % -1 -> 0
119 -> 120 4.85 % 0 -> 0

Excited State: 4
2.8622 eV 433.17 nm 23086.cm-1 f=0.0006
114 -> 120 75.60 % -5 -> 0
117 -> 120 16.67 % -2 -> 0

Excited State: 5
3.0392 eV 407.94 nm 24513.cm-1 f=0.0751
115 -> 120 2.59 % -4 -> 0
116 -> 120 85.56 % -3 -> 0
119 -> 120 2.90 % 0 -> 0

Excited State: 6
3.1042 eV 399.41 nm 25037.cm-1 f=0.0047
113 -> 120 7.16 % -6 -> 0
115 -> 120 80.97 % -4 -> 0

Excited State: 7
3.5794 eV 346.38 nm 28870.cm-1 f=0.0087
112 -> 122 2.51 % -7 -> 2
113 -> 120 18.15 % -6 -> 0
114 -> 122 5.14 % -5 -> 2
115 -> 120 3.06 % -4 -> 0
117 -> 122 52.96 % -2 -> 2
119 -> 123 2.08 % 0 -> 3

Excited State: 8
3.5839 eV 345.95 nm 28906.cm-1 f=0.0002
108 -> 122 4.65 % -11 -> 2
110 -> 120 2.36 % -9 -> 0
112 -> 120 9.68 % -7 -> 0
116 -> 122 15.93 % -3 -> 2
118 -> 122 21.87 % -1 -> 2
119 -> 122 33.49 % 0 -> 2

Excited State: 9
3.6635 eV 338.43 nm 29548.cm-1 f=0.0001
110 -> 120 2.36 % -9 -> 0
112 -> 120 79.78 % -7 -> 0
114 -> 120 2.00 % -5 -> 0
118 -> 122 5.18 % -1 -> 2
119 -> 122 4.39 % 0 -> 2

Excited State: 10
3.6859 eV 336.38 nm 29728.cm-1 f=0.0280
109 -> 120 4.90 % -10 -> 0
111 -> 120 2.40 % -8 -> 0
113 -> 120 54.35 % -6 -> 0
114 -> 122 2.37 % -5 -> 2
115 -> 120 3.89 % -4 -> 0
117 -> 122 14.83 % -2 -> 2
119 -> 123 4.56 % 0 -> 3

Excited State: 11
3.7759 eV 328.35 nm 30455.cm-1 f=0.0001
108 -> 122 3.43 % -11 -> 2
109 -> 122 2.03 % -10 -> 2
111 -> 122 10.86 % -8 -> 2
113 -> 122 2.97 % -6 -> 2
116 -> 122 8.22 % -3 -> 2
118 -> 122 48.62 % -1 -> 2
119 -> 122 13.19 % 0 -> 2

Excited State: 12
3.8851 eV 319.13 nm 31335.cm-1 f=0.0191
111 -> 120 83.77 % -8 -> 0
119 -> 123 4.30 % 0 -> 3

Excited State: 13
4.0103 eV 309.16 nm 32346.cm-1 f=0.0404
111 -> 120 2.17 % -8 -> 0
119 -> 121 89.42 % 0 -> 1

Excited State: 14
4.0851 eV 303.51 nm 32948.cm-1 f=0.0000
110 -> 120 86.44 % -9 -> 0
112 -> 120 3.90 % -7 -> 0
119 -> 122 5.15 % 0 -> 2

Excited State: 15
4.1309 eV 300.14 nm 33318.cm-1 f=0.0157
109 -> 120 29.23 % -10 -> 0
110 -> 122 10.03 % -9 -> 2
112 -> 122 2.53 % -7 -> 2
119 -> 121 4.38 % 0 -> 1
119 -> 123 40.51 % 0 -> 3

Excited State: 16
4.1586 eV 298.14 nm 33541.cm-1 f=0.0260
104 -> 122 2.31 % -15 -> 2
107 -> 122 3.58 % -12 -> 2
109 -> 120 7.36 % -10 -> 0
110 -> 122 45.70 % -9 -> 2
112 -> 122 18.55 % -7 -> 2
114 -> 122 5.37 % -5 -> 2
119 -> 123 6.15 % 0 -> 3

Excited State: 17
4.2674 eV 290.54 nm 34419.cm-1 f=0.0002
109 -> 122 6.76 % -10 -> 2
110 -> 120 4.31 % -9 -> 0
111 -> 122 4.54 % -8 -> 2
115 -> 122 3.84 % -4 -> 2
116 -> 122 29.75 % -3 -> 2
117 -> 121 2.89 % -2 -> 1
119 -> 122 40.34 % 0 -> 2

Excited State: 18
4.2779 eV 289.83 nm 34503.cm-1 f=0.0520
108 -> 120 22.45 % -11 -> 0
109 -> 120 36.07 % -10 -> 0
113 -> 120 6.65 % -6 -> 0
119 -> 123 20.94 % 0 -> 3

Excited State: 19
4.3234 eV 286.77 nm 34871.cm-1 f=0.0002
114 -> 121 2.31 % -5 -> 1
117 -> 121 89.61 % -2 -> 1

Excited State: 20
4.4143 eV 280.87 nm 35604.cm-1 f=0.0380
118 -> 121 78.89 % -1 -> 1

Excited State: 21
4.5043 eV 275.26 nm 36329.cm-1 f=0.0484
108 -> 120 58.99 % -11 -> 0
109 -> 120 9.24 % -10 -> 0
119 -> 123 4.54 % 0 -> 3
119 -> 124 10.56 % 0 -> 4
119 -> 125 3.59 % 0 -> 5

Excited State: 22
4.6049 eV 269.24 nm 37142.cm-1 f=0.0175
108 -> 120 8.70 % -11 -> 0
119 -> 123 5.87 % 0 -> 3
119 -> 124 65.41 % 0 -> 4

Excited State: 23
4.6967 eV 263.98 nm 37882.cm-1 f=0.0004
112 -> 121 69.33 % -7 -> 1
112 -> 123 2.11 % -7 -> 3
114 -> 121 21.85 % -5 -> 1

Excited State: 24
4.7147 eV 262.97 nm 38027.cm-1 f=0.0379
115 -> 123 2.62 % -4 -> 3
116 -> 121 2.07 % -3 -> 1
116 -> 123 3.53 % -3 -> 3
118 -> 123 29.18 % -1 -> 3
119 -> 124 2.50 % 0 -> 4
119 -> 125 49.29 % 0 -> 5

Excited State: 25
4.7669 eV 260.10 nm 38447.cm-1 f=0.0000
104 -> 120 4.07 % -15 -> 0
107 -> 120 87.76 % -12 -> 0

Excited State: 26
4.7855 eV 259.08 nm 38598.cm-1 f=0.0006
115 -> 123 5.38 % -4 -> 3
118 -> 123 60.59 % -1 -> 3
119 -> 124 2.55 % 0 -> 4
119 -> 125 16.81 % 0 -> 5

Excited State: 27
4.8004 eV 258.28 nm 38718.cm-1 f=0.0022
114 -> 120 2.30 % -5 -> 0
114 -> 123 20.76 % -5 -> 3
117 -> 123 63.01 % -2 -> 3
117 -> 124 2.77 % -2 -> 4

Excited State: 28
4.8700 eV 254.59 nm 39279.cm-1 f=0.0427
111 -> 121 2.20 % -8 -> 1
115 -> 121 7.86 % -4 -> 1
116 -> 121 74.04 % -3 -> 1

Excited State: 29
4.9177 eV 252.12 nm 39664.cm-1 f=0.0001
108 -> 122 4.71 % -11 -> 2
109 -> 122 4.45 % -10 -> 2
111 -> 122 28.46 % -8 -> 2
113 -> 122 17.71 % -6 -> 2
115 -> 122 20.80 % -4 -> 2
116 -> 122 6.74 % -3 -> 2
118 -> 122 9.74 % -1 -> 2

Excited State: 30
4.9432 eV 250.82 nm 39869.cm-1 f=0.0029
114 -> 121 2.31 % -5 -> 1
114 -> 123 56.61 % -5 -> 3
114 -> 124 3.26 % -5 -> 4
117 -> 123 25.45 % -2 -> 3

Figure S1. In the following picture, some Kohn-Sham orbitals of (NR)Pd(acac) (**1a**) are reported that are relevant in describing the low-energy electronic transitions discussed in the paper.

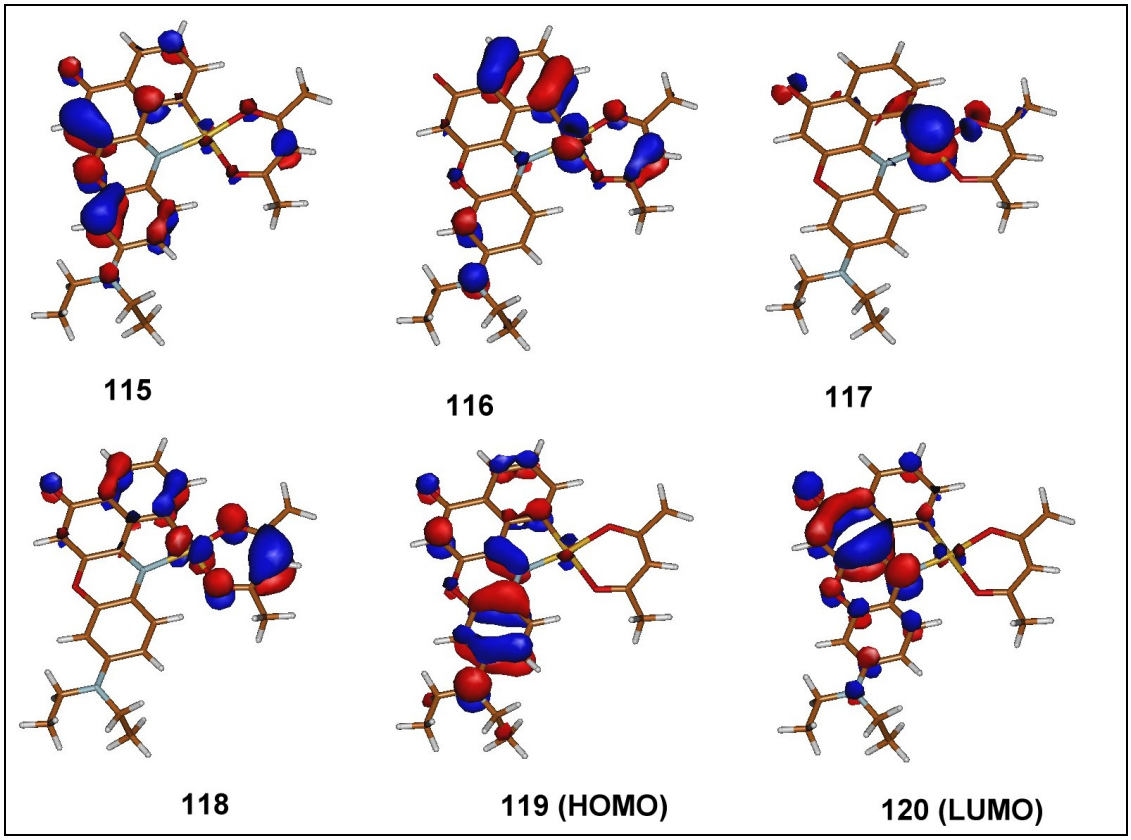


Table S2. Optimized structure of (NR)Pd(acac) (**1a**). Cartesian coordinates in Angstrom.

C	1.765516	-1.000956	-0.119004
C	1.205165	0.285752	-0.089304
C	2.109621	1.367693	-0.095700
C	3.483357	1.192773	-0.135518
C	4.043923	-0.102994	-0.185296
C	3.132105	-1.195038	-0.159750
O	1.671906	2.659866	-0.055020
C	0.336432	2.897747	-0.012318
C	-0.568624	1.766385	-0.008891
N	-0.164473	0.511347	-0.044836
C	-1.978532	2.012885	0.037944
C	-2.494828	3.317392	0.078377
C	-1.562644	4.478857	0.072963
C	-0.128025	4.173091	0.026030
C	-3.879419	3.484982	0.123513
C	-4.703040	2.355982	0.127407
C	-4.170782	1.056548	0.087014
C	-2.790690	0.864466	0.041452
Pd	-1.783801	-0.822582	-0.023264
O	-3.529499	-1.819202	0.012814
C	-3.681425	-3.085327	-0.013796
C	-2.672544	-4.058664	-0.072530
C	-1.288538	-3.801224	-0.111981
O	-0.742710	-2.655847	-0.099778
O	-1.965826	5.640161	0.106556
N	5.406099	-0.289093	-0.275896
H	0.562831	5.010493	0.022416
H	-4.288534	4.490517	0.154763
H	-5.783196	2.483523	0.162537
H	-4.835274	0.196858	0.091222
H	4.087850	2.090646	-0.118008
H	3.494285	-2.215980	-0.173979
H	1.094146	-1.852468	-0.108459
C	5.974667	-1.605442	-0.025861
C	6.264958	0.890602	-0.187010
C	-0.333899	-4.970983	-0.175593
H	-2.987383	-5.095467	-0.088889
C	-5.124544	-3.527577	0.024261
C	7.743692	0.641483	-0.449557
H	5.918593	1.613296	-0.934811
H	6.151236	1.374345	0.796566
H	8.258261	1.607500	-0.435196
H	8.212756	0.011802	0.312514
H	7.912442	0.190481	-1.432810
H	6.980705	-1.627423	-0.447605
C	6.029429	-1.996856	1.452888
H	5.411434	-2.349716	-0.595346
H	6.460254	-2.997994	1.565455
H	6.649839	-1.295959	2.021584
H	5.030893	-2.001901	1.900447
H	-0.847528	-5.934538	-0.179715
H	0.277504	-4.886515	-1.080507
H	0.343960	-4.929184	0.683776
H	-5.228731	-4.614045	-0.003436
H	-5.594802	-3.142837	0.935304
H	-5.657029	-3.091733	-0.827552

(NR)Pt(acac) (2a)

Table S3. Computed singlet excited states of (NR)Pt(acac) (**2a**). The following text lists the energy (in eV and nm), the oscillator strengths and percentage composition of the most important monoelectronic excitations for each excited state. Excited States composition has been expressed in two ways. The first one uses the Kohn-Sham orbital numerical label of the occupied and virtual orbital as produced by the computation (for instance, 119 -> 120 for the HOMO -> LUMO transition when the HOMO is the 119th orbital and the LUMO is the 120th one). The second way assign the "0" label to the HOMO, the "–1" label to the HOMO-1 orbital and so on, the "0" label to the LUMO, "1" to LUMO+1 and so on (thus, 0 -> 0 is the HOMO -> LUMO transition, -2 -> 1 is the HOMO-2 -> LUMO+1 transition).

Excited State: 1
2.2728 eV 545.51 nm 18331.cm-1 f=0.2568
117 -> 120 4.95 % -2 -> 0
118 -> 120 15.25 % -1 -> 0
119 -> 120 63.77 % 0 -> 0

Excited State: 2
2.7365 eV 453.07 nm 22072.cm-1 f=0.0016
114 -> 120 26.41 % -5 -> 0
116 -> 120 67.29 % -3 -> 0

Excited State: 3
2.7555 eV 449.95 nm 22225.cm-1 f=0.2418
118 -> 120 67.43 % -1 -> 0
119 -> 120 12.51 % 0 -> 0

Excited State: 4
2.8089 eV 441.40 nm 22655.cm-1 f=0.0007
114 -> 120 63.90 % -5 -> 0
116 -> 120 29.67 % -3 -> 0

Excited State: 5
2.9466 eV 420.77 nm 23766.cm-1 f=0.1108
117 -> 120 85.74 % -2 -> 0
118 -> 120 4.04 % -1 -> 0
119 -> 120 2.06 % 0 -> 0

Excited State: 6
3.0782 eV 402.78 nm 24827.cm-1 f=0.0083
113 -> 120 4.59 % -6 -> 0
115 -> 120 85.73 % -4 -> 0

Excited State: 7
3.5288 eV 351.35 nm 28462.cm-1 f=0.0000
112 -> 120 92.87 % -7 -> 0

Excited State: 8
3.6618 eV 338.58 nm 29535.cm-1 f=0.0087
109 -> 120 2.12 % -10 -> 0
110 -> 120 2.14 % -9 -> 0
111 -> 120 3.90 % -8 -> 0
113 -> 120 73.44 % -6 -> 0
115 -> 120 5.11 % -4 -> 0
119 -> 122 6.00 % 0 -> 2

Excited State: 9
3.7789 eV 328.10 nm 30479.cm-1 f=0.0422
118 -> 121 3.63 % -1 -> 1
119 -> 121 93.01 % 0 -> 1

Excited State: 10
3.8773 eV 319.77 nm 31272.cm-1 f=0.0242
111 -> 120 81.43 % -8 -> 0
113 -> 120 2.93 % -6 -> 0
119 -> 122 7.07 % 0 -> 2

Excited State: 11
4.0668 eV 304.87 nm 32801.cm-1 f=0.0091
109 -> 120 2.16 % -10 -> 0
110 -> 120 3.61 % -9 -> 0
116 -> 125 2.28 % -3 -> 5
118 -> 121 75.88 % -1 -> 1
119 -> 121 2.66 % 0 -> 1
119 -> 122 3.51 % 0 -> 2

Excited State: 12
4.1215 eV 300.82 nm 33242.cm-1 f=0.0012
109 -> 120 39.17 % -10 -> 0
110 -> 120 52.32 % -9 -> 0

Excited State: 13
4.1338 eV 299.93 nm 33341.cm-1 f=0.0728
109 -> 120 18.96 % -10 -> 0
110 -> 120 7.03 % -9 -> 0
111 -> 120 5.95 % -8 -> 0
118 -> 121 6.76 % -1 -> 1
119 -> 122 48.45 % 0 -> 2

Excited State: 14
4.1989 eV 295.28 nm 33866.cm-1 f=0.0001
114 -> 121 2.19 % -5 -> 1
116 -> 121 94.97 % -3 -> 1

Excited State: 15
4.2445 eV 292.11 nm 34234.cm-1 f=0.0476
108 -> 120 16.98 % -11 -> 0
109 -> 120 25.44 % -10 -> 0
110 -> 120 22.68 % -9 -> 0
113 -> 120 6.30 % -6 -> 0
119 -> 122 16.01 % 0 -> 2

Excited State: 16
4.3735 eV 283.49 nm 35275.cm-1 f=0.0002
117 -> 125 10.47 % -2 -> 5
118 -> 125 25.14 % -1 -> 5
118 -> 126 2.49 % -1 -> 6
119 -> 125 43.52 % 0 -> 5
119 -> 126 2.85 % 0 -> 6

Excited State: 17
4.4803 eV 276.73 nm 36136.cm-1 f=0.0027
108 -> 120 23.57 % -11 -> 0
116 -> 125 9.32 % -3 -> 5
117 -> 121 32.27 % -2 -> 1
119 -> 123 14.19 % 0 -> 3
119 -> 124 2.60 % 0 -> 4

Excited State: 18
4.4883 eV 276.24 nm 36200.cm-1 f=0.0901
108 -> 120 32.10 % -11 -> 0
116 -> 125 28.68 % -3 -> 5
116 -> 126 2.15 % -3 -> 6
117 -> 121 7.60 % -2 -> 1
118 -> 122 8.64 % -1 -> 2
119 -> 122 2.53 % 0 -> 2

Excited State: 19
4.5851 eV 270.41 nm 36981.cm-1 f=0.0004
108 -> 125 2.06 % -11 -> 5
111 -> 125 2.90 % -8 -> 5
112 -> 121 22.92 % -7 -> 1
114 -> 121 8.73 % -5 -> 1
117 -> 125 10.16 % -2 -> 5
118 -> 125 30.27 % -1 -> 5

118 -> 126 2.22 % -1 -> 6
119 -> 125 7.18 % 0 -> 5

Excited State: 20
4.5908 eV 270.07 nm 37027.cm-1 f=0.0151
108 -> 120 7.67 % -11 -> 0
116 -> 125 16.32 % -3 -> 5
117 -> 122 2.64 % -2 -> 2
118 -> 122 8.99 % -1 -> 2
119 -> 122 3.43 % 0 -> 2
119 -> 123 37.40 % 0 -> 3
119 -> 124 3.95 % 0 -> 4

Excited State: 21
4.6220 eV 268.25 nm 37279.cm-1 f=0.0117
116 -> 125 7.88 % -3 -> 5
117 -> 121 14.17 % -2 -> 1
118 -> 122 24.50 % -1 -> 2
119 -> 123 25.00 % 0 -> 3
119 -> 124 12.82 % 0 -> 4

Excited State: 22
4.6453 eV 266.90 nm 37467.cm-1 f=0.0002
109 -> 121 2.32 % -10 -> 1
110 -> 121 2.18 % -9 -> 1
112 -> 121 38.65 % -7 -> 1
114 -> 121 17.55 % -5 -> 1
117 -> 125 4.80 % -2 -> 5
118 -> 125 17.62 % -1 -> 5
119 -> 125 4.32 % 0 -> 5

Excited State: 23
4.6679 eV 265.61 nm 37649.cm-1 f=0.0289
108 -> 120 8.43 % -11 -> 0
116 -> 125 8.90 % -3 -> 5
116 -> 126 2.78 % -3 -> 6
117 -> 121 26.34 % -2 -> 1
118 -> 122 33.12 % -1 -> 2
119 -> 124 4.64 % 0 -> 4

Excited State: 24
4.7322 eV 262.00 nm 38168.cm-1 f=0.0141
115 -> 121 2.27 % -4 -> 1
115 -> 122 8.81 % -4 -> 2
116 -> 125 2.37 % -3 -> 5
117 -> 122 4.43 % -2 -> 2
118 -> 122 15.02 % -1 -> 2
119 -> 124 46.37 % 0 -> 4
119 -> 127 2.15 % 0 -> 7

Excited State: 25
4.8446 eV 255.92 nm 39075.cm-1 f=0.0009
114 -> 120 3.17 % -5 -> 0
114 -> 122 54.29 % -5 -> 2
114 -> 123 4.32 % -5 -> 3
116 -> 122 26.57 % -3 -> 2

Excited State: 26
4.9525 eV 250.35 nm 39944.cm-1 f=0.0051
107 -> 120 6.92 % -12 -> 0
114 -> 122 22.62 % -5 -> 2
116 -> 122 59.95 % -3 -> 2

Excited State: 27
4.9571 eV 250.12 nm 39981.cm-1 f=0.0530
115 -> 121 82.20 % -4 -> 1
117 -> 121 5.84 % -2 -> 1
117 -> 122 3.14 % -2 -> 2
119 -> 124 3.54 % 0 -> 4

Excited State: 28
4.9907 eV 248.43 nm 40253.cm-1 f=0.0655
112 -> 125 3.65 % -7 -> 5
115 -> 121 4.63 % -4 -> 1
115 -> 122 2.46 % -4 -> 2
117 -> 122 70.77 % -2 -> 2
119 -> 123 2.54 % 0 -> 3

Excited State: 29
4.9998 eV 247.98 nm 40326.cm-1 f=0.0011
104 -> 120 3.61 % -15 -> 0
107 -> 120 80.71 % -12 -> 0
116 -> 122 5.85 % -3 -> 2

Excited State: 30
5.0102 eV 247.47 nm 40409.cm-1 f=0.0042
109 -> 125 6.43 % -10 -> 5
110 -> 125 6.03 % -9 -> 5
112 -> 125 52.64 % -7 -> 5
112 -> 126 5.64 % -7 -> 6
114 -> 125 9.63 % -5 -> 5
117 -> 122 5.46 % -2 -> 2

Figure S4. In the following picture, some (NR)Pt(acac) (**2a**) Kohn-Sham orbitals are reported that are relevant in describing the low-energy electronic transitions discussed in the paper.

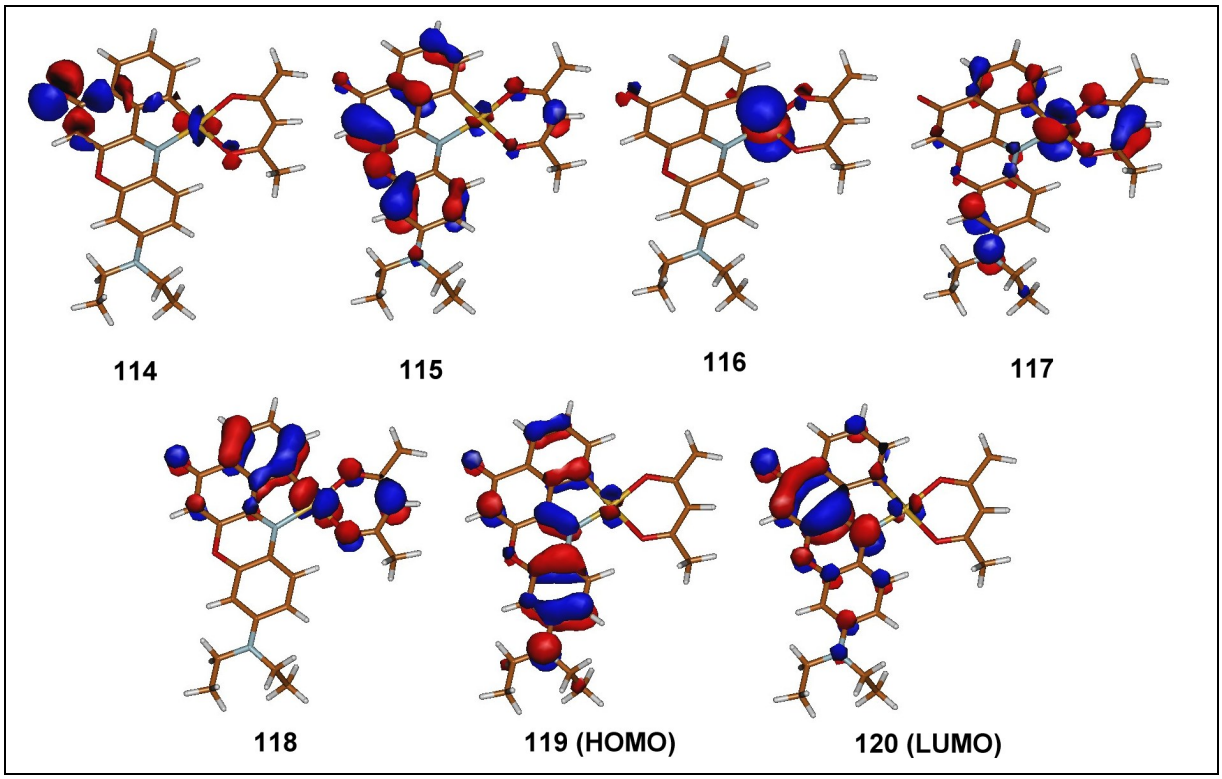


Table S4. Optimized structure of (NR)Pt(acac) (**2a**). Cartesian coordinates in Angstrom.

C	1.915098	-0.959086	-0.107534
C	1.378617	0.336863	-0.086349
C	2.306553	1.398765	-0.100836
C	3.676671	1.193687	-0.141884
C	4.212397	-0.111773	-0.183552
C	3.277723	-1.182575	-0.148345
O	1.905122	2.702479	-0.067316
C	0.576948	2.973810	-0.019615
C	-0.357074	1.869737	-0.008824
N	0.009536	0.597215	-0.041314
C	-1.755066	2.152873	0.042314
C	-2.241720	3.468397	0.081177
C	-1.281196	4.605684	0.067491
C	0.144641	4.261145	0.015583
C	-3.621165	3.663028	0.132660
C	-4.465072	2.546608	0.144097
C	-3.960642	1.238346	0.104754
C	-2.580892	1.012543	0.052574
Pt	-1.596206	-0.694988	-0.017199
O	-3.341024	-1.685908	0.018967
C	-3.518245	-2.952798	-0.013082
C	-2.527380	-3.939865	-0.079631
C	-1.141206	-3.701433	-0.121896
O	-0.581885	-2.560680	-0.105163
O	-1.653089	5.777682	0.098439
N	5.571166	-0.326399	-0.276766
H	0.857735	5.079581	0.005762
H	-4.012710	4.675510	0.162933
H	-5.542337	2.695203	0.184429

H	-4.645575	0.394977	0.114582
H	4.297687	2.080288	-0.130489
H	3.616830	-2.211524	-0.156087
H	1.231629	-1.799388	-0.091643
C	6.112983	-1.648114	0.002837
C	6.452531	0.836993	-0.198333
C	-0.197349	-4.877089	-0.194380
H	-2.858110	-4.971552	-0.100335
C	-4.969205	-3.358656	0.028019
C	7.923866	0.558561	-0.473179
H	6.113609	1.562521	-0.946547
H	6.356429	1.327394	0.783982
H	8.456239	1.514992	-0.475379
H	8.389767	-0.070884	0.291025
H	8.073354	0.093090	-1.452846
H	7.118059	-1.700384	-0.418802
C	6.160670	-2.007816	1.489850
H	5.534355	-2.393316	-0.549651
H	6.571955	-3.014434	1.624664
H	6.794844	-1.306963	2.043247
H	5.162257	-1.983577	1.937158
H	-0.720695	-5.835250	-0.203102
H	0.412767	-4.793249	-1.100124
H	0.482330	-4.847162	0.663960
H	-5.096698	-4.442255	-0.006271
H	-5.427257	-2.969986	0.943566
H	-5.495204	-2.905853	-0.818895

(NR)Pd(hfacac) (1b)

Table S5. Computed singlet excited states of (NR)Pd(hfacac) (**1b**). The following text lists the energy (in eV and nm), the oscillator strengths and percentage composition of the most important monoelectronic excitations for each excited state.

Excited States composition has been expressed in two ways. The first one uses the Kohn-Sham orbital numerical label of the occupied and virtual orbital as produced by the computation (for instance, 119 -> 120 for the HOMO -> LUMO transition when the HOMO is the 119th orbital and the LUMO is the 120th one). The second way assign the "0" label to the HOMO, the "–1" label to the HOMO-1 orbital and so on, the "0" label to the LUMO, "1" to LUMO+1 and so on (thus, 0 -> 0 is the HOMO -> LUMO transition, -2 -> 1 is the HOMO-2 -> LUMO+1 transition).

Excited State: 1
2.3792 eV 521.12 nm 19189.cm-1 f=0.4334
142 -> 144 4.78 % -1 -> 0
143 -> 144 72.58 % 0 -> 0

Excited State: 2
2.7689 eV 447.78 nm 22332.cm-1 f=0.0001
139 -> 144 12.55 % -4 -> 0
140 -> 144 78.21 % -3 -> 0

Excited State: 3
2.8924 eV 428.66 nm 23329.cm-1 f=0.0098
143 -> 145 98.62 % 0 -> 1

Excited State: 4
3.0112 eV 411.75 nm 24287.cm-1 f=0.0741
138 -> 144 5.25 % -5 -> 0
141 -> 144 3.50 % -2 -> 0
142 -> 144 76.37 % -1 -> 0

Excited State: 5
3.0283 eV 409.42 nm 24425.cm-1 f=0.0445
141 -> 144 84.62 % -2 -> 0
142 -> 144 3.83 % -1 -> 0

Excited State: 6
3.0807 eV 402.45 nm 24848.cm-1 f=0.0015
139 -> 144 82.39 % -4 -> 0
140 -> 144 14.62 % -3 -> 0

Excited State: 7
3.3386 eV 371.37 nm 26927.cm-1 f=0.0001
134 -> 146 2.30 % -9 -> 2
138 -> 146 3.28 % -5 -> 2
141 -> 146 5.56 % -2 -> 2
142 -> 146 15.92 % -1 -> 2
143 -> 146 65.54 % 0 -> 2

Excited State: 8
3.3921 eV 365.51 nm 27359.cm-1 f=0.0368
138 -> 144 56.49 % -5 -> 0
139 -> 146 17.92 % -4 -> 2
140 -> 146 10.24 % -3 -> 2
142 -> 144 4.23 % -1 -> 0

Excited State: 9
3.5236 eV 351.87 nm 28420.cm-1 f=0.0208
138 -> 144 21.97 % -5 -> 0
139 -> 146 23.48 % -4 -> 2
140 -> 146 8.24 % -3 -> 2
142 -> 145 26.41 % -1 -> 1

Excited State: 10
3.5469 eV 349.56 nm 28607.cm-1 f=0.0002
139 -> 145 56.92 % -4 -> 1
140 -> 145 39.24 % -3 -> 1

Excited State: 11
3.6700 eV 337.83 nm 29601.cm-1 f=0.0250
138 -> 144 5.65 % -5 -> 0
139 -> 146 12.90 % -4 -> 2
140 -> 146 4.93 % -3 -> 2
141 -> 145 6.41 % -2 -> 1
142 -> 145 58.12 % -1 -> 1

Excited State: 12
3.6784 eV 337.06 nm 29668.cm-1 f=0.0002
132 -> 146 9.04 % -11 -> 2
137 -> 146 2.07 % -6 -> 2
138 -> 146 9.35 % -5 -> 2
142 -> 146 52.73 % -1 -> 2
143 -> 146 13.78 % 0 -> 2

Excited State: 13
3.7271 eV 332.66 nm 30061.cm-1 f=0.0156
136 -> 144 13.52 % -7 -> 0
137 -> 144 73.91 % -6 -> 0
143 -> 147 3.43 % 0 -> 3

Excited State: 14
3.9776 eV 311.71 nm 32081.cm-1 f=0.0014
136 -> 144 25.71 % -7 -> 0
137 -> 144 2.06 % -6 -> 0
138 -> 145 2.02 % -5 -> 1
141 -> 145 43.31 % -2 -> 1
142 -> 145 2.74 % -1 -> 1
143 -> 147 17.87 % 0 -> 3

Excited State: 15
3.9919 eV 310.59 nm 32197.cm-1 f=0.0163
136 -> 144 21.67 % -7 -> 0
141 -> 145 43.35 % -2 -> 1
142 -> 145 3.09 % -1 -> 1
143 -> 147 24.85 % 0 -> 3

Excited State: 16
3.9942 eV 310.41 nm 32215.cm-1 f=0.0001
134 -> 146 18.80 % -9 -> 2
135 -> 144 5.45 % -8 -> 0
137 -> 146 6.86 % -6 -> 2
138 -> 146 30.36 % -5 -> 2
141 -> 146 9.16 % -2 -> 2
143 -> 146 16.70 % 0 -> 2

Excited State: 17
4.1198 eV 300.95 nm 33228.cm-1 f=0.0001
135 -> 144 56.01 % -8 -> 0
135 -> 145 14.56 % -8 -> 1
138 -> 146 3.17 % -5 -> 2
139 -> 145 4.81 % -4 -> 1
140 -> 145 6.58 % -3 -> 1

Excited State: 18
4.1310 eV 300.13 nm 33319.cm-1 f=0.0044
133 -> 146 41.73 % -10 -> 2
135 -> 146 38.24 % -8 -> 2
140 -> 146 4.55 % -3 -> 2

Excited State: 19
4.1639 eV 297.76 nm 33584.cm-1 f=0.0465
134 -> 144 2.00 % -9 -> 0
134 -> 145 3.20 % -9 -> 1

135 -> 144 4.20 % -8 -> 0
135 -> 145 2.18 % -8 -> 1
138 -> 145 67.93 % -5 -> 1
141 -> 145 3.06 % -2 -> 1
142 -> 145 2.29 % -1 -> 1
143 -> 147 2.62 % 0 -> 3

Excited State: 20
4.1768 eV 296.84 nm 33688.cm-1 f=0.0061
133 -> 144 2.38 % -10 -> 0
135 -> 144 24.12 % -8 -> 0
135 -> 145 27.73 % -8 -> 1
138 -> 145 6.10 % -5 -> 1
139 -> 145 14.55 % -4 -> 1
140 -> 145 18.64 % -3 -> 1

Excited State: 21
4.2716 eV 290.25 nm 34453.cm-1 f=0.1050
136 -> 144 30.42 % -7 -> 0
137 -> 144 9.57 % -6 -> 0
138 -> 145 2.93 % -5 -> 1
143 -> 147 35.17 % 0 -> 3
143 -> 149 4.69 % 0 -> 5

Excited State: 22
4.4018 eV 281.67 nm 35503.cm-1 f=0.0178
132 -> 144 3.78 % -11 -> 0
134 -> 144 80.04 % -9 -> 0
137 -> 145 3.26 % -6 -> 1
138 -> 145 2.69 % -5 -> 1

Excited State: 23
4.4631 eV 277.80 nm 35997.cm-1 f=0.0003
133 -> 144 4.59 % -10 -> 0
133 -> 145 3.89 % -10 -> 1
135 -> 145 38.07 % -8 -> 1
139 -> 145 18.82 % -4 -> 1
140 -> 145 31.02 % -3 -> 1

Excited State: 24
4.5641 eV 271.65 nm 36812.cm-1 f=0.0003
133 -> 144 82.75 % -10 -> 0
135 -> 144 3.66 % -8 -> 0
135 -> 145 4.22 % -8 -> 1
137 -> 145 2.01 % -6 -> 1

Excited State: 25
4.5696 eV 271.32 nm 36857.cm-1 f=0.0168
134 -> 144 3.27 % -9 -> 0
136 -> 145 2.31 % -7 -> 1
137 -> 145 79.00 % -6 -> 1
138 -> 145 3.00 % -5 -> 1

Excited State: 26
4.5762 eV 270.94 nm 36909.cm-1 f=0.0021
141 -> 150 2.16 % -2 -> 6
143 -> 147 2.60 % 0 -> 3
143 -> 148 68.34 % 0 -> 4
143 -> 149 8.97 % 0 -> 5

Excited State: 27
4.6456 eV 266.89 nm 37469.cm-1 f=0.0000
137 -> 146 3.99 % -6 -> 2
138 -> 146 20.34 % -5 -> 2
141 -> 146 66.68 % -2 -> 2
142 -> 146 8.09 % -1 -> 2

Excited State: 28
4.7056 eV 263.48 nm 37954.cm-1 f=0.0348
132 -> 144 3.24 % -11 -> 0
141 -> 147 12.79 % -2 -> 3
143 -> 148 12.74 % 0 -> 4
143 -> 149 58.11 % 0 -> 5
143 -> 150 2.26 % 0 -> 6

Excited State: 29
4.7418 eV 261.47 nm 38245.cm-1 f=0.0003
130 -> 145 2.72 % -13 -> 1
133 -> 145 86.25 % -10 -> 1
135 -> 145 4.40 % -8 -> 1

Excited State: 30
4.7727 eV 259.78 nm 38494.cm-1 f=0.0190
132 -> 144 81.91 % -11 -> 0
134 -> 144 3.27 % -9 -> 0
143 -> 149 2.17 % 0 -> 5

Figure S3. In the following picture, some (NR)Pd(hfacac) (**1b**) Kohn-Sham orbitals are reported that are relevant in describing the low-energy electronic transitions discussed in the paper.

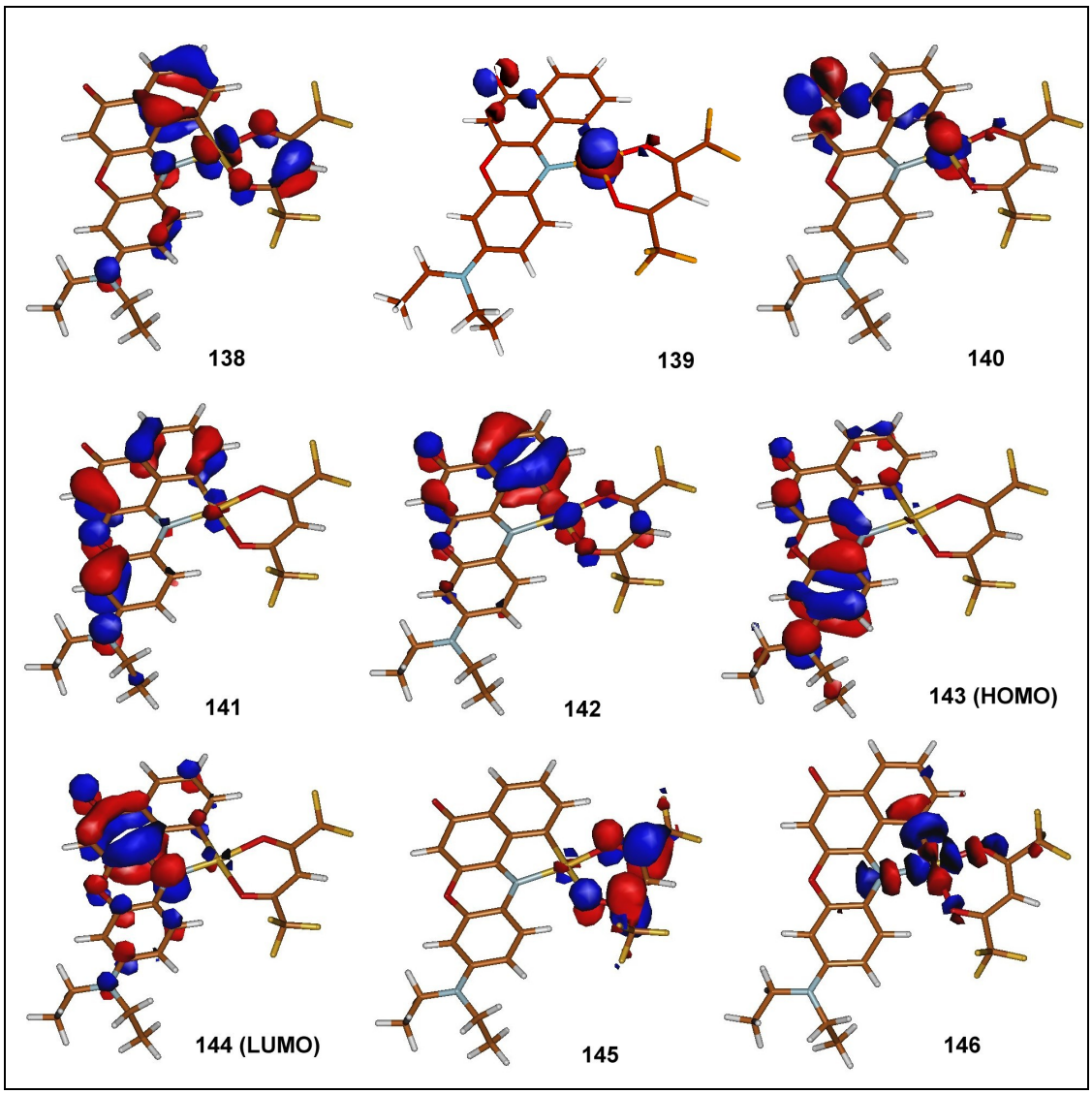


Table S6. Optimized structure of (NR)Pd(hfacac) (**1b**). Cartesian coordinates in Angstrom.

C	2.133342	-0.892541	-0.066744
C	1.921101	0.494450	-0.077333
C	3.076724	1.304751	-0.106919
C	4.356872	0.777574	-0.134387
C	4.565534	-0.619919	-0.143273
C	3.401481	-1.436261	-0.092451
O	2.997341	2.667390	-0.101774
C	1.774248	3.250630	-0.055525
C	0.603649	2.402815	-0.030052
N	0.657215	1.079796	-0.044425
C	-0.686673	3.010248	0.018155
C	-0.848082	4.402525	0.041529
C	0.356369	5.278175	0.012316
C	1.659817	4.603964	-0.037248
C	-2.142646	4.918193	0.093776
C	-3.226746	4.034853	0.120970
C	-3.048463	2.642607	0.097024
C	-1.761043	2.103181	0.045162
Pd	-1.206265	0.213017	-0.009271
O	-3.140891	-0.357235	0.044459
C	-3.594750	-1.538915	0.026981
C	-2.910642	-2.751745	-0.038449
C	-1.512857	-2.815515	-0.097402
O	-0.685728	-1.869054	-0.093904
O	0.272556	6.504124	0.029040
N	5.830332	-1.153958	-0.215538
H	2.546307	5.230119	-0.058715
H	-2.283907	5.994745	0.112693
H	-4.237977	4.433723	0.161850
H	-3.916449	1.989949	0.118636
H	5.172534	1.489224	-0.136830
H	3.482111	-2.516219	-0.074068
H	1.276639	-1.551455	-0.035385
C	6.036393	-2.567607	0.069344
C	6.966723	-0.234809	-0.162451
C	-0.842792	-4.198763	-0.198699
H	-3.480402	-3.670217	-0.045422
C	-5.131909	-1.557615	0.096371
C	8.329383	-0.865920	-0.410876
H	6.814960	0.528267	-0.934575
H	6.985991	0.292531	0.804764
H	9.075572	-0.065254	-0.426700
H	8.624180	-1.569075	0.373810
H	8.371672	-1.377216	-1.377955
H	7.005899	-2.858544	-0.337128
C	5.974772	-2.922160	1.556714
H	5.304112	-3.153553	-0.492789
H	6.130929	-3.997377	1.696601
H	6.750006	-2.391080	2.119155
H	5.004495	-2.659116	1.988547
F	-1.712305	-5.207016	-0.064495
F	-0.241462	-4.329036	-1.389443
F	0.093133	-4.332444	0.749772
F	-5.629378	-2.799210	0.033104
F	-5.547578	-1.005520	1.242438
F	-5.650847	-0.853512	-0.915309

(NR)Pt(hfacac) (2b)

Table S6. Computed singlet excited states of (NR)Pt(hfacac) (**2b**). The following text lists the energy (in eV and nm), the oscillator strengths and percentage composition of the most important monoelectronic excitations for each excited state.
Excited States composition has been expressed in two ways. The first one uses the Kohn-Sham orbital numerical label of the occupied and virtual orbital as produced by the computation (for instance, 119 -> 120 for the HOMO -> LUMO transition when the HOMO is the 119th orbital and the LUMO is the 120th one). The second way assign the "0" label to the HOMO, the "–1" label to the HOMO-1 orbital and so on, the "0" label to the LUMO, "1" to LUMO+1 and so on (thus, 0 -> 0 is the HOMO -> LUMO transition, -2 -> 1 is the HOMO-2 -> LUMO+1 transition).

Excited State: 1
2.2987 eV 539.38 nm 18540.cm-1 f=0.3585
142 -> 144 10.26 % -1 -> 0
143 -> 144 69.82 % 0 -> 0

Excited State: 2
2.7035 eV 458.60 nm 21805.cm-1 f=0.0235
143 -> 145 97.15 % 0 -> 1

Excited State: 3
2.7358 eV 453.19 nm 22066.cm-1 f=0.0000
138 -> 144 7.35 % -5 -> 0
140 -> 144 82.89 % -3 -> 0
140 -> 146 2.16 % -3 -> 2

Excited State: 4
2.8333 eV 437.60 nm 22852.cm-1 f=0.1478
139 -> 144 3.00 % -4 -> 0
141 -> 144 2.63 % -2 -> 0
142 -> 144 73.77 % -1 -> 0
143 -> 144 7.14 % 0 -> 0

Excited State: 5
2.9691 eV 417.58 nm 23948.cm-1 f=0.0219
137 -> 144 2.55 % -6 -> 0
139 -> 144 4.46 % -4 -> 0
141 -> 144 83.38 % -2 -> 0

Excited State: 6
3.0382 eV 408.08 nm 24505.cm-1 f=0.0018
138 -> 144 88.89 % -5 -> 0
140 -> 144 8.61 % -3 -> 0

Excited State: 7
3.2277 eV 384.12 nm 26034.cm-1 f=0.0021
139 -> 144 20.95 % -4 -> 0
142 -> 145 66.56 % -1 -> 1

Excited State: 8
3.3159 eV 373.90 nm 26745.cm-1 f=0.1147
139 -> 144 60.60 % -4 -> 0
141 -> 144 2.10 % -2 -> 0
142 -> 144 2.37 % -1 -> 0
142 -> 145 24.24 % -1 -> 1

Excited State: 9
3.3864 eV 366.12 nm 27313.cm-1 f=0.0001
138 -> 145 77.63 % -5 -> 1
140 -> 145 21.01 % -3 -> 1

Excited State: 10
3.6975 eV 335.32 nm 29822.cm-1 f=0.0182
136 -> 144 10.10 % -7 -> 0
137 -> 144 75.90 % -6 -> 0
141 -> 145 2.06 % -2 -> 1
143 -> 146 2.08 % 0 -> 2

Excited State: 11
3.7341 eV 332.03 nm 30118.cm-1 f=0.0387
137 -> 144 3.09 % -6 -> 0
139 -> 145 10.76 % -4 -> 1
141 -> 145 76.39 % -2 -> 1

Excited State: 12
3.8878 eV 318.91 nm 31357.cm-1 f=0.0005
135 -> 144 79.73 % -8 -> 0
135 -> 145 5.01 % -8 -> 1
140 -> 145 4.77 % -3 -> 1

Excited State: 13
3.9066 eV 317.37 nm 31509.cm-1 f=0.0261
135 -> 144 2.91 % -8 -> 0
139 -> 145 70.76 % -4 -> 1
141 -> 145 16.73 % -2 -> 1
142 -> 145 2.42 % -1 -> 1

Excited State: 14
3.9785 eV 311.63 nm 32089.cm-1 f=0.0001
135 -> 144 9.30 % -8 -> 0
135 -> 145 34.82 % -8 -> 1
138 -> 145 9.86 % -5 -> 1
140 -> 145 38.49 % -3 -> 1

Excited State: 15
3.9952 eV 310.33 nm 32224.cm-1 f=0.0246
136 -> 144 40.77 % -7 -> 0
143 -> 146 50.31 % 0 -> 2

Excited State: 16
4.1314 eV 300.10 nm 33322.cm-1 f=0.0002
135 -> 144 3.33 % -8 -> 0
139 -> 147 2.49 % -4 -> 3
141 -> 147 2.75 % -2 -> 3
142 -> 147 21.49 % -1 -> 3
143 -> 147 61.07 % 0 -> 3

Excited State: 17
4.2586 eV 291.14 nm 34348.cm-1 f=0.0804
134 -> 144 6.99 % -9 -> 0
136 -> 144 34.28 % -7 -> 0
137 -> 144 6.68 % -6 -> 0
137 -> 145 2.88 % -6 -> 1
143 -> 146 28.41 % 0 -> 2
143 -> 149 4.41 % 0 -> 5

Excited State: 18
4.2956 eV 288.63 nm 34646.cm-1 f=0.0004
135 -> 145 51.94 % -8 -> 1
138 -> 145 9.26 % -5 -> 1
140 -> 145 32.84 % -3 -> 1

Excited State: 19
4.3503 eV 285.00 nm 35088.cm-1 f=0.0265
134 -> 144 60.97 % -9 -> 0
136 -> 144 5.81 % -7 -> 0
137 -> 145 17.09 % -6 -> 1
143 -> 146 3.63 % 0 -> 2
143 -> 148 2.14 % 0 -> 4

Excited State: 20
4.3874 eV 282.59 nm 35387.cm-1 f=0.0298
134 -> 144 12.84 % -9 -> 0

137 -> 145 40.46 % -6 -> 1
138 -> 147 27.30 % -5 -> 3
139 -> 145 3.45 % -4 -> 1
140 -> 147 5.05 % -3 -> 3

Excited State: 21
4.4593 eV 278.04 nm 35966.cm-1 f=0.0040
132 -> 144 2.63 % -11 -> 0
134 -> 144 5.29 % -9 -> 0
137 -> 145 28.22 % -6 -> 1
138 -> 147 42.10 % -5 -> 3
140 -> 147 7.68 % -3 -> 3

Excited State: 22
4.4680 eV 277.49 nm 36037.cm-1 f=0.0003
132 -> 147 4.32 % -11 -> 3
133 -> 144 3.12 % -10 -> 0
133 -> 145 7.16 % -10 -> 1
137 -> 147 2.31 % -6 -> 3
139 -> 147 8.76 % -4 -> 3
142 -> 147 49.79 % -1 -> 3
143 -> 147 13.92 % 0 -> 3

Excited State: 23
4.5330 eV 273.51 nm 36562.cm-1 f=0.0005
133 -> 144 39.00 % -10 -> 0
133 -> 145 40.53 % -10 -> 1
135 -> 145 2.83 % -8 -> 1
142 -> 147 6.39 % -1 -> 3
143 -> 147 2.67 % 0 -> 3

Excited State: 24
4.5804 eV 270.68 nm 36944.cm-1 f=0.0016
143 -> 146 2.96 % 0 -> 2
143 -> 148 71.32 % 0 -> 4
143 -> 149 6.03 % 0 -> 5

Excited State: 25
4.6645 eV 265.80 nm 37622.cm-1 f=0.0004
133 -> 144 47.99 % -10 -> 0
133 -> 145 39.57 % -10 -> 1

Excited State: 26
4.6963 eV 264.00 nm 37879.cm-1 f=0.0523
139 -> 146 2.17 % -4 -> 2
141 -> 146 10.23 % -2 -> 2
142 -> 146 3.93 % -1 -> 2
143 -> 148 9.24 % 0 -> 4
143 -> 149 59.96 % 0 -> 5
143 -> 150 2.92 % 0 -> 6

Excited State: 27
4.7839 eV 259.17 nm 38585.cm-1 f=0.0068
132 -> 144 51.95 % -11 -> 0
136 -> 145 15.01 % -7 -> 1
142 -> 146 23.75 % -1 -> 2

Excited State: 28
4.8138 eV 257.56 nm 38826.cm-1 f=0.0109
134 -> 145 5.63 % -9 -> 1
136 -> 145 62.89 % -7 -> 1
141 -> 146 3.40 % -2 -> 2
142 -> 146 20.03 % -1 -> 2

Excited State: 29
4.8279 eV 256.81 nm 38939.cm-1 f=0.0001
138 -> 146 6.86 % -5 -> 2
140 -> 144 3.04 % -3 -> 0
140 -> 146 73.43 % -3 -> 2
140 -> 148 3.56 % -3 -> 4

Excited State: 30
4.8525 eV 255.51 nm 39137.cm-1 f=0.0352
132 -> 144 26.98 % -11 -> 0
134 -> 144 3.31 % -9 -> 0
134 -> 145 9.38 % -9 -> 1
136 -> 145 12.38 % -7 -> 1
142 -> 146 31.72 % -1 -> 2

Figure S4. In the following picture, some (NR)Pt(hfacac) (**2b**) Kohn-Sham orbitals are reported that are relevant in describing the low-energy electronic transitions discussed in the paper.

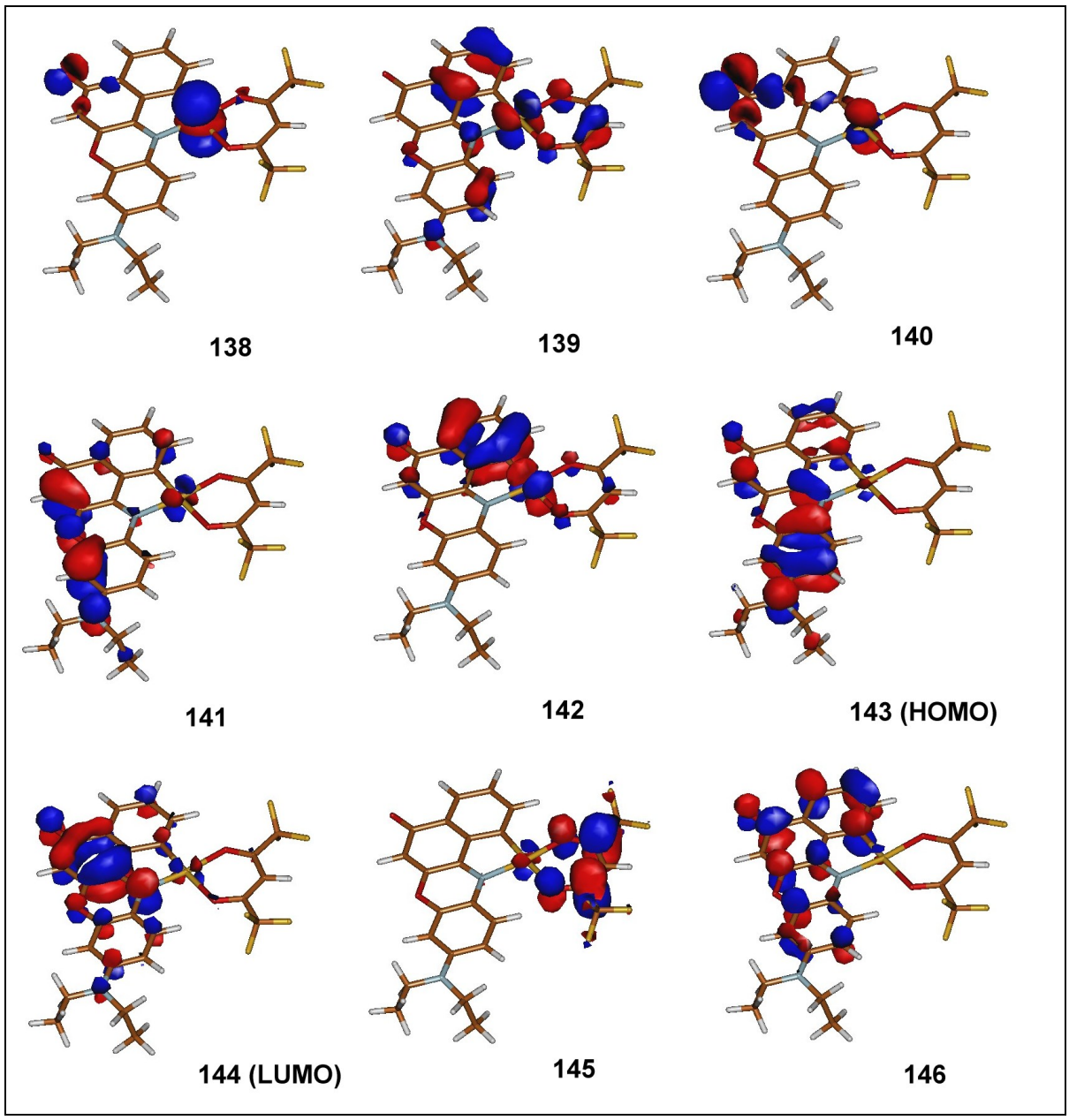


Table S8. Optimized structure of (NR)Pt(hfacac) (**2b**). Cartesian coordinates in Angstrom.

C	2.133342	-0.892541	-0.066744
C	1.921101	0.494450	-0.077333
C	3.076724	1.304751	-0.106919
C	4.356872	0.777574	-0.134387
C	4.565534	-0.619919	-0.143273
C	3.401481	-1.436261	-0.092451
O	2.997341	2.667390	-0.101774
C	1.774248	3.250630	-0.055525
C	0.603649	2.402815	-0.030052
N	0.657215	1.079796	-0.044425
C	-0.686673	3.010248	0.018155
C	-0.848082	4.402525	0.041529
C	0.356369	5.278175	0.012316
C	1.659817	4.603964	-0.037248
C	-2.142646	4.918193	0.093776
C	-3.226746	4.034853	0.120970
C	-3.048463	2.642607	0.097024
C	-1.761043	2.103181	0.045162
Pt	-1.206265	0.213017	-0.009271
O	-3.140891	-0.357235	0.044459
C	-3.594750	-1.538915	0.026981
C	-2.910642	-2.751745	-0.038449
C	-1.512857	-2.815515	-0.097402
O	-0.685728	-1.869054	-0.093904
O	0.272556	6.504124	0.029040
N	5.830332	-1.153958	-0.215538
H	2.546307	5.230119	-0.058715
H	-2.283907	5.994745	0.112693
H	-4.237977	4.433723	0.161850
H	-3.916449	1.989949	0.118636
H	5.172534	1.489224	-0.136830
H	3.482111	-2.516219	-0.074068
H	1.276639	-1.551455	-0.035385
C	6.036393	-2.567607	0.069344
C	6.966723	-0.234809	-0.162451
C	-0.842792	-4.198763	-0.198699
H	-3.480402	-3.670217	-0.045422
C	-5.131909	-1.557615	0.096371
C	8.329383	-0.865920	-0.410876
H	6.814960	0.528267	-0.934575
H	6.985991	0.292531	0.804764
H	9.075572	-0.065254	-0.426700
H	8.624180	-1.569075	0.373810
H	8.371672	-1.377216	-1.377955
H	7.005899	-2.858544	-0.337128
C	5.974772	-2.922160	1.556714
H	5.304112	-3.153553	-0.492789
H	6.130929	-3.997377	1.696601
H	6.750006	-2.391080	2.119155
H	5.004495	-2.659116	1.988547
F	-1.712305	-5.207016	-0.064495
F	-0.241462	-4.329036	-1.389443
F	0.093133	-4.332444	0.749772
F	-5.629378	-2.799210	0.033104
F	-5.547578	-1.005520	1.242438
F	-5.650847	-0.853512	-0.915309

Photophysical Results

Figure S5. Emission spectra of **1a**, **2a**, **1b** and **2b** in CH_2Cl_2 solution.

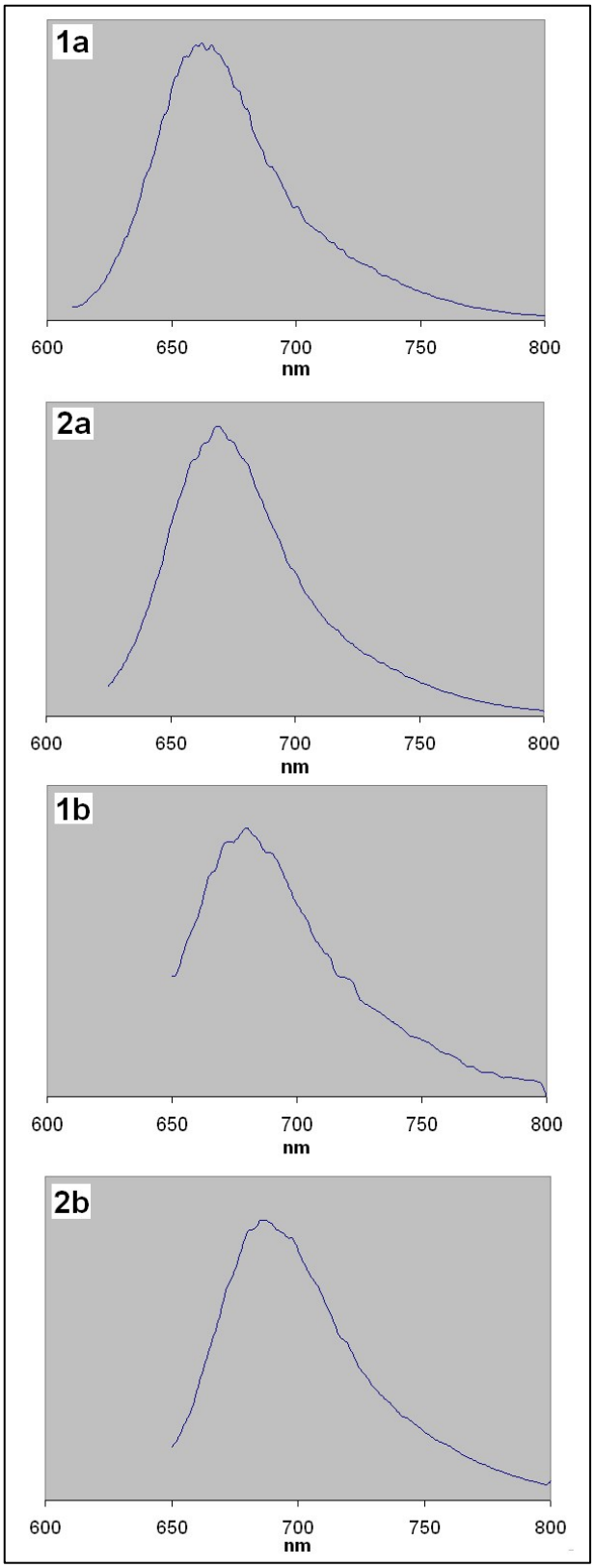
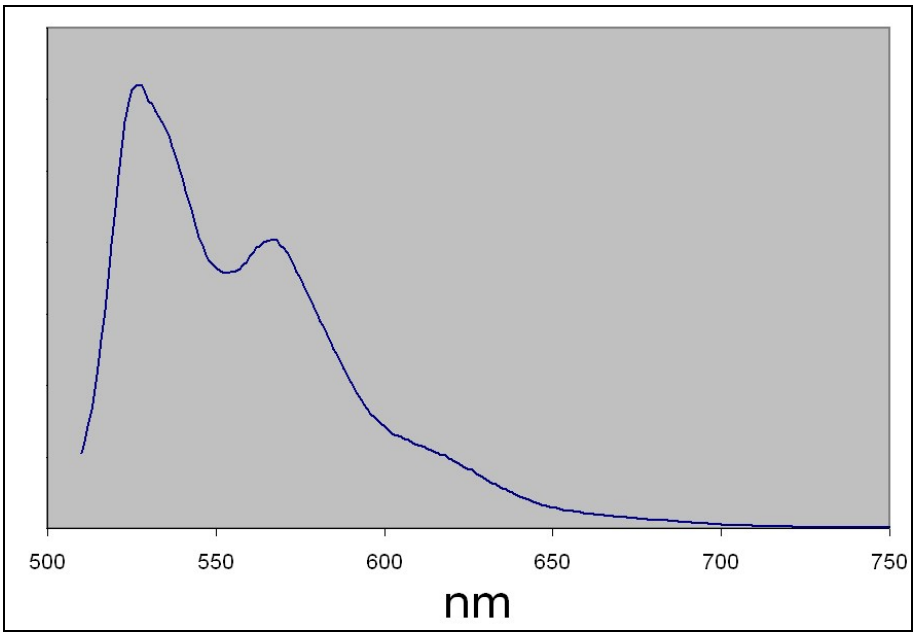


Figure S6. Emission spectrum of HNR in C_6H_{12} solution.



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