

Electronic Supplementary Information for:

Long-lived Emissive Intra-ligand Triplet Excited States (³IL): Next Generation Luminescent Oxygen Sensing Scheme and a Case Study With Red Phosphorescent Diimine Pt(II) Bis(acetylide) Complexes Containing Ethynylated Naphthalimide or Pyrene Subunits

Huimin Guo,* Shaomin Ji, Wanhua Wu, Wenting Wu, Jingyin Shao, and Jianzhang Zhao*

^a State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, 158 Zhongshan Road, Dalian 116012 P. R. China.

E-mail: zhaojzh@dlut.edu.cn ; guohm@dlut.edu.cn

General information.....	S2
Figure S1. ¹ H NMR of Pt-1	S3
Figure S2. ¹³ C NMR of Pt-1	S3
Figure S3. TOF ESI MS of Pt-1	S4
Figure S4. ¹ H NMR of Pt-2	S4
Figure S5. TOF ESI MS of Pt-2	S5
Figure S6. ¹ H NMR of Pt-3	S5
Figure S7. ¹³ C NMR of Pt-3	S6
Figure S8. Emission intensity changes of the complexes at different concentrations in acetonitrile.....	S7
Figure S9. Oxygen sensing properties of complexes Pt-1	S8
Figure S10. Oxygen sensing properties of complexes PtOEP	S8
Figure S11. Two-sites model plots for sensing films of Pt-1 and PtOEP in polymer IMPEK-C.....	S9
Figure S12. Emission spectra of complexes Pt-1 , Pt-2 and Pt-3 in IMPEK-C films under N ₂ and O ₂	S10
Z-matrix of Pt-1	S11
Z-matrix of Pt-2	S21
Z-matrix of Pt-3	S29

Experimental section

General information

NMR spectra were taken on a 400 MHz Varian Unity Inova spectrophotometer. Mass spectra were recorded with a Q-TOF Micro MS spectrometer. UV-Vis spectra were taken on a HP8453 UV-visible spectrophotometer. Fluorescence spectra were recorded on a JASCO FP-6500 or a Sanco 970 CRT spectrofluorometer. Luminescence quantum yields were measured with Ru(bpy)₂(Phen) as the reference ($\phi = 6.0\%$ in acetonitrile). Emission decay measurements at RT was performed with a pulsed diode laser (PicoQuant GmbH Model LDH-P-C-375, $\lambda_{\text{ex}} = 372\text{ nm}$, pulse width 100 ps), attached to the fluorescence spectrophotometer (Jobin Yvon Fluorolog 3).

The structures of the complexes were optimized using density functional theory (DFT) with B3LYP functional and 6-31G(d)/LanL2DZ basis set. The excited state related calculations were carried out with the time dependent DFT (TD-DFT) with the ground state geometry. The 6-31G(d) basis set was employed for C, H, N, O, S and the LanL2DZ basis set was used for Ru(II). There are no imaginary frequencies for all optimized structures. All these calculations were performed with Gaussian 09 (M. J. Frisch, Trucks, et al, Gaussian 09, Revision A. I., Gaussian, Inc., Wallingford CT, 2009.).

Synthesis of Complexes Pt-1, Pt-2 and Pt-3.

All the compounds were synthesized according to reported method (Pomestchenko, I. E.; Luman, C. R.; Hissler, M.; Ziessel, R.; Castellano, F. N. *Inorg. Chem.*, 2003, 42(5), 1394-1396). For the detail synthesis of Pt-1, please refer to our recent paper (H. Guo, M. L. Muro-Small, S. Ji, J. Zhao and F.N. Castellano. *Inorg. Chem.*, **2010**, DOI:10.1021/ic101107b.).

For **Pt-1**, ¹H NMR (400 MHz, CDCl₃): δ 9.68 (d, $J = 6.0\text{ Hz}$, 2H), 9.14 (d, $J = 8.0\text{ Hz}$, 2H), 8.51 (t, $J = 7.6\text{ Hz}$, 4H), 8.05 (s, 2H), 7.88 (d, $J = 7.6\text{ Hz}$, 2H), 7.68 (d, $J = 5.2\text{ Hz}$, 2H), 7.48 (t, $J = 8.0\text{ Hz}$, 2H), 4.16 (t, $J = 7.6\text{ Hz}$, 4H), 1.71 (m, 4H), 1.48 (m, 24H), 0.96 (t, $J = 7.6\text{ Hz}$, 4H). ¹³C NMR (100 MHz, CDCl₃): δ 164.63, 164.43, 156.40, 151.45, 134.26, 33.26, 133.15, 131.24, 130.99, 130.10, 128.52, 126.64, 125.19, 122.90, 119.60, 119.26, 101.55, 100.12, 40.34, 36.16, 30.44, 20.61, 14.03. HR-MALDI-MS: C₅₄H₅₆NaN₄Pt, Calculated $m/z = 1038.3534$, found, $m/z = 1038.3608$.

For **Pt-2**, ¹H NMR (400 MHz, d₆-acetone): δ 9.64 (d, $J = 5.6\text{ Hz}$, 2H), 8.60 (s, 2H), 7.85 (d, $J = 6.0\text{ Hz}$, 2H), 7.35 (d, $J = 6.8\text{ Hz}$, 4H), 7.19 (t, $J = 8.0\text{ Hz}$, 4H), 7.07 (t, $J = 7.6\text{ Hz}$, 2H), 1.44 (s, 18H). HR-MALDI-MS: C₃₄H₃₄N₂Pt, Calculated, $m/z = 665.2370$, found $m/z = 665.2318$.

For **Pt-3**, ¹H NMR (400 MHz, CDCl₃): δ 9.95 (d, $J = 6.0\text{ Hz}$, 2H), 9.19 (d, $J = 9.2\text{ Hz}$, 2H), 8.29 (d, $J = 8.0\text{ Hz}$, 2H), 8.09 (d, $J = 7.6\text{ Hz}$, 4H), 8.01 (m, 10H), 7.91 (t, $J = 7.6\text{ Hz}$, 2H), 7.62 (d, $J = 6.0\text{ Hz}$, 2H), 1.45 (s, 18H). ¹³C NMR (100 MHz, CDCl₃): δ 163.73, 156.53, 151.65, 132.53, 131.77, 131.73, 130.40, 129.43, 128.48, 128.03, 127.82, 127.64, 127.29, 126.66, 125.82, 124.97, 124.75, 124.54, 124.50, 124.11, 118.99, 101.31, 93.74, 30.48, 29.90.

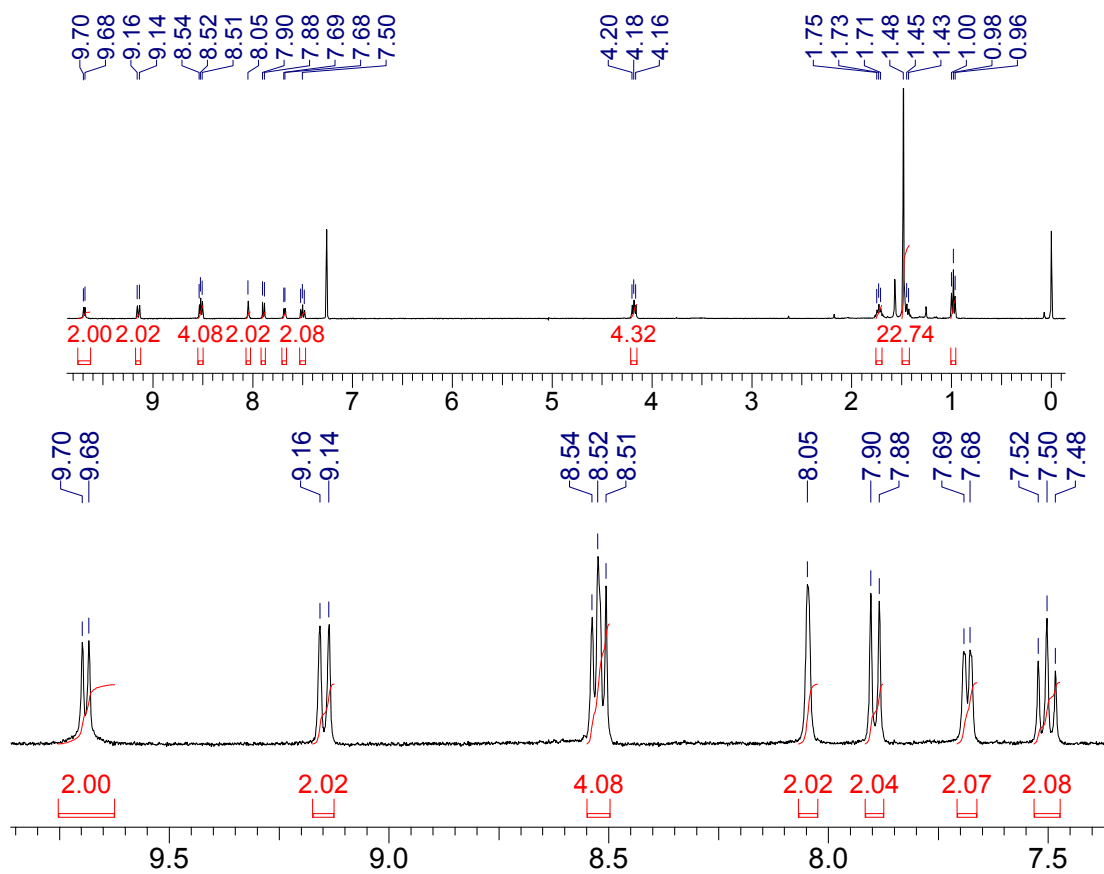


Figure S1. ^1H NMR of Pt-1 (CDCl_3 , 400 MHz).

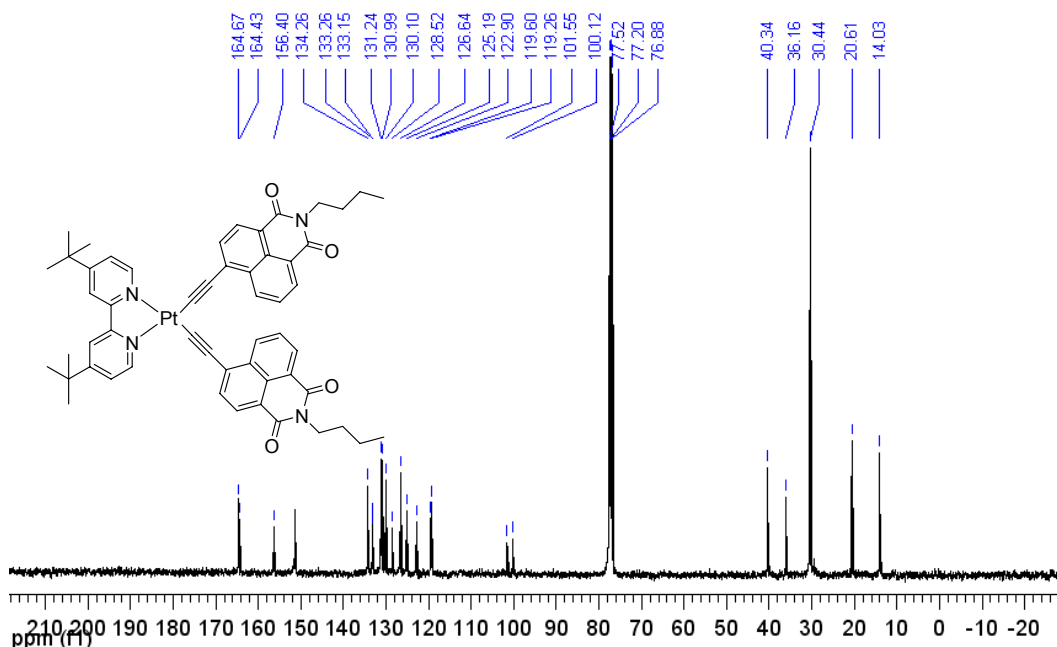


Figure S2. ^{13}C NMR of Pt-1 (CDCl_3 , 100 MHz).

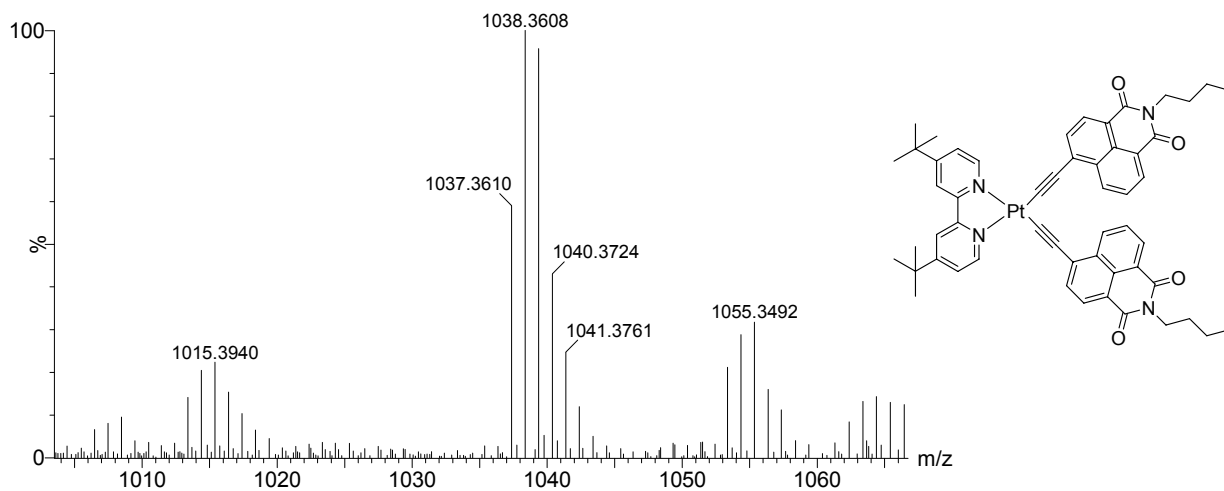


Figure S3. HR-MALDI-MS of Pt-1.

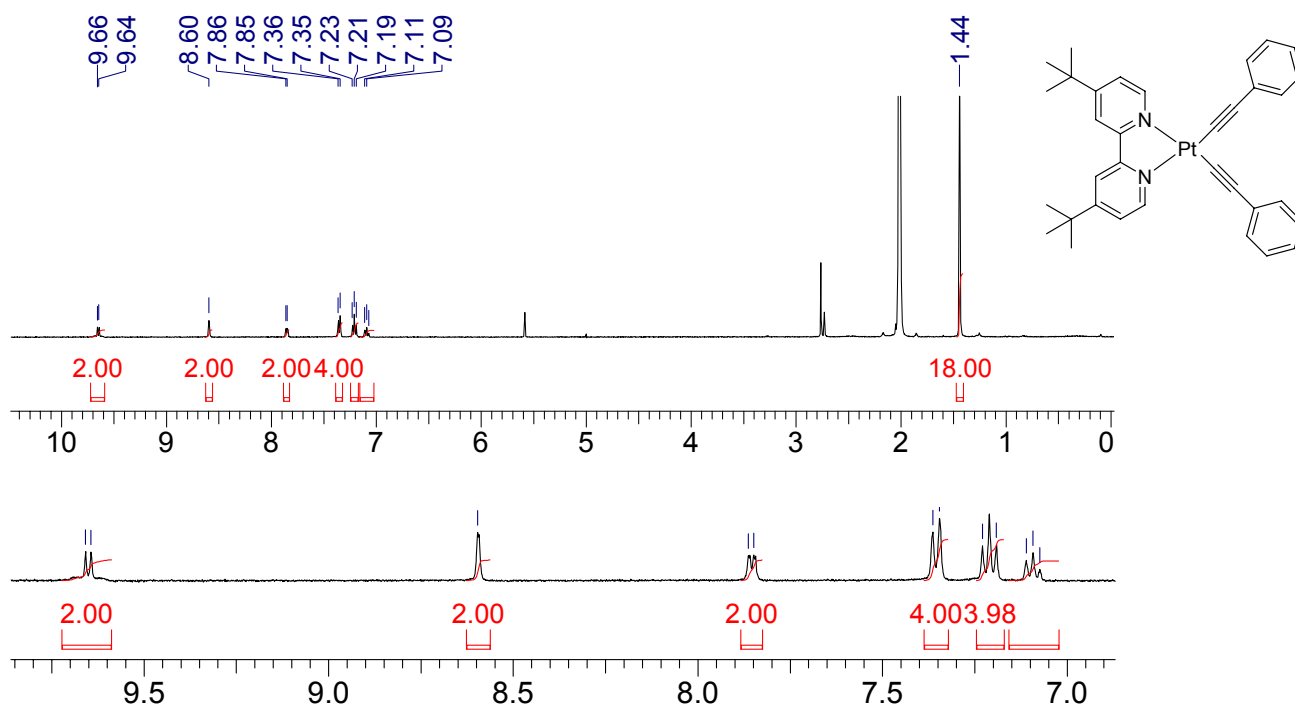


Figure S4. ^1H NMR of Pt-2 (d_6 -acetone, 400MHz).

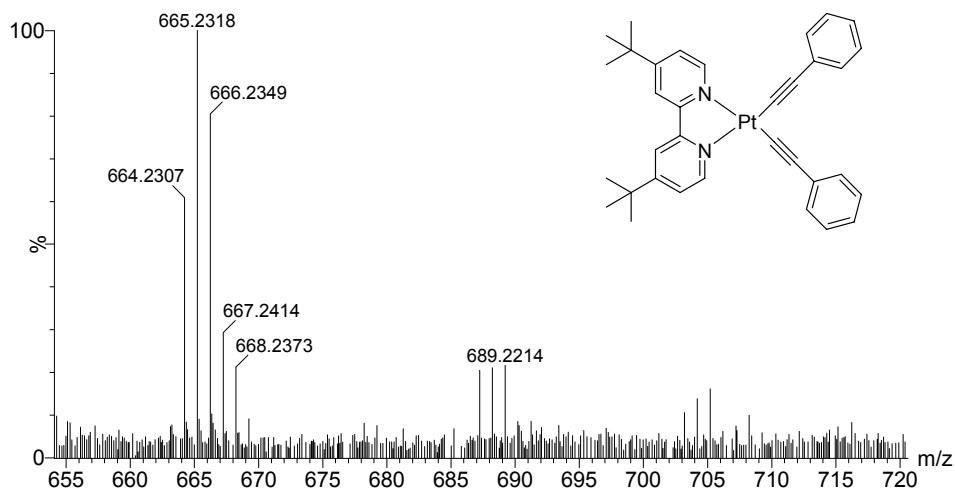


Figure S5. FR-MALDI-MS of Pt-2.

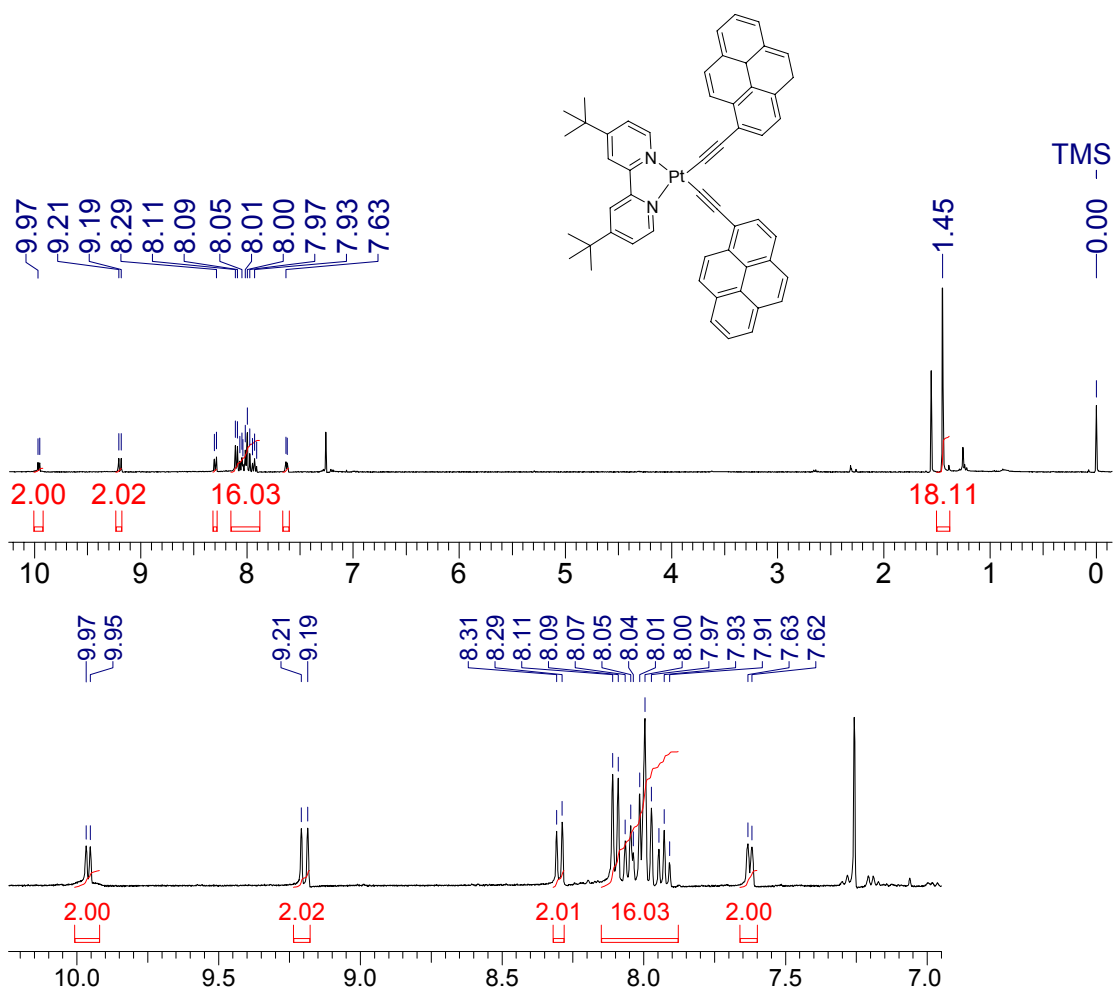


Figure S6. ^1H NMR of Pt-3 (CDCl_3 , 400 MHz).

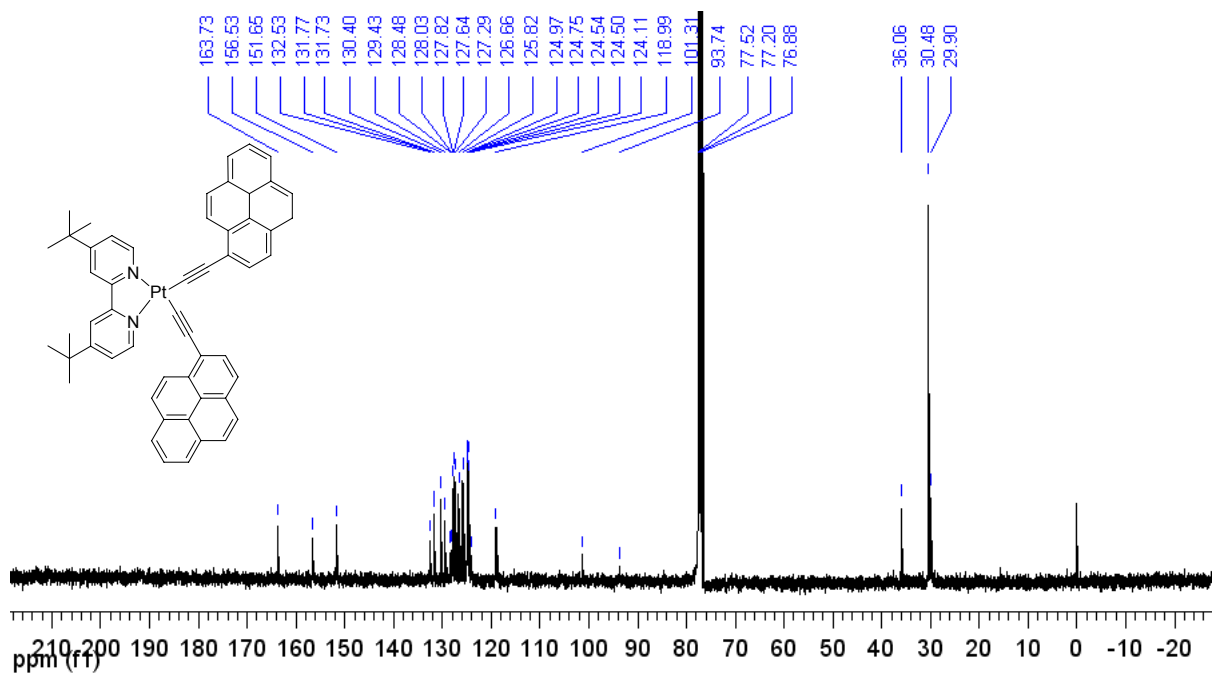


Figure S7. ^{13}C NMR of Pt-3 (CDCl_3 , 100 MHz).

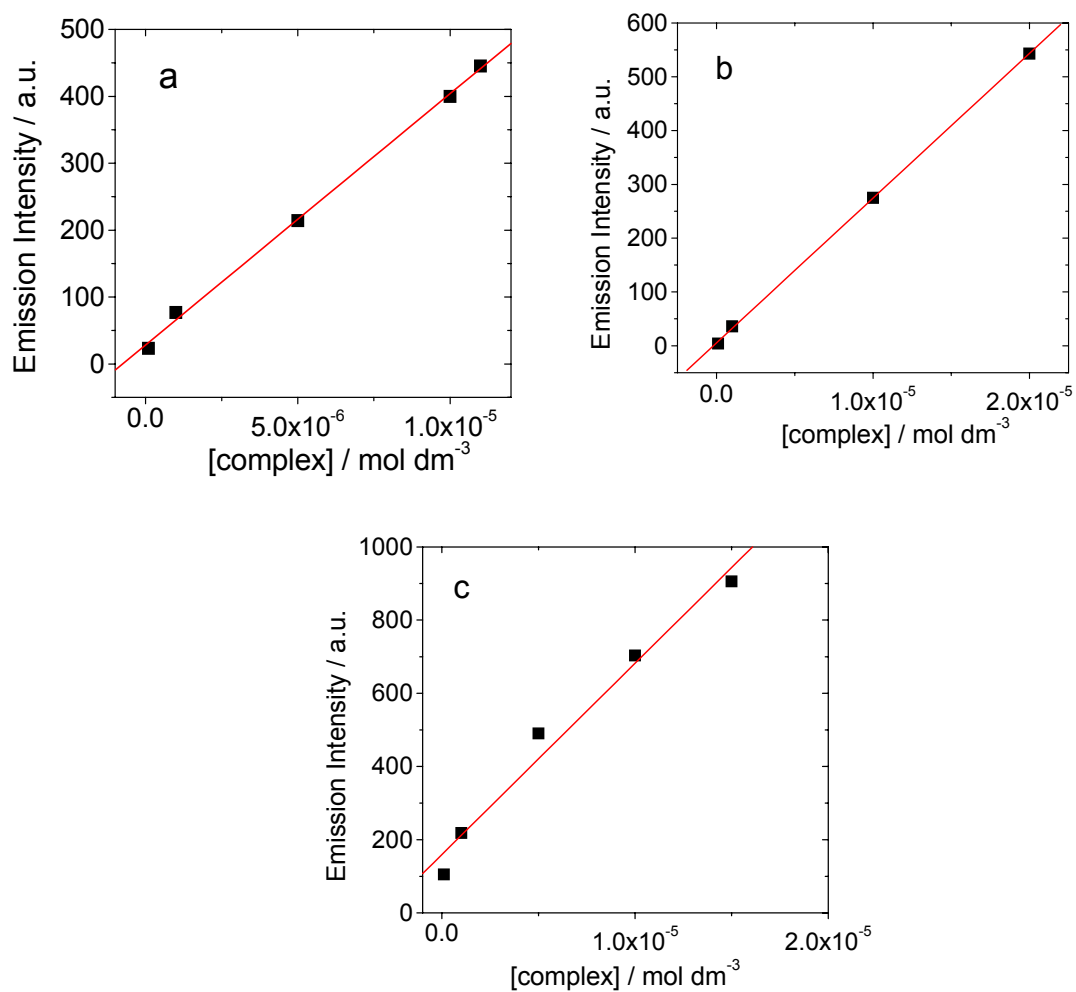
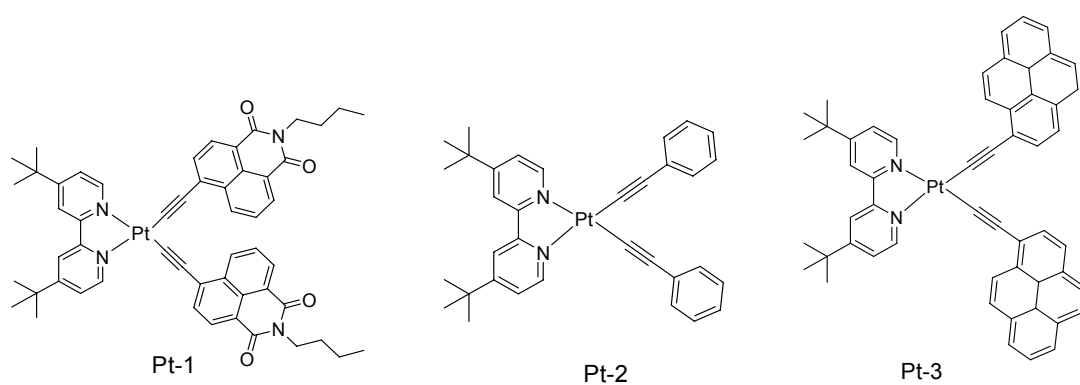


Figure S8. Emission intensity changes of **Pt-1**, **Pt-2** and **Pt-3** with different concentrations in acetonitrile. 25 °C.



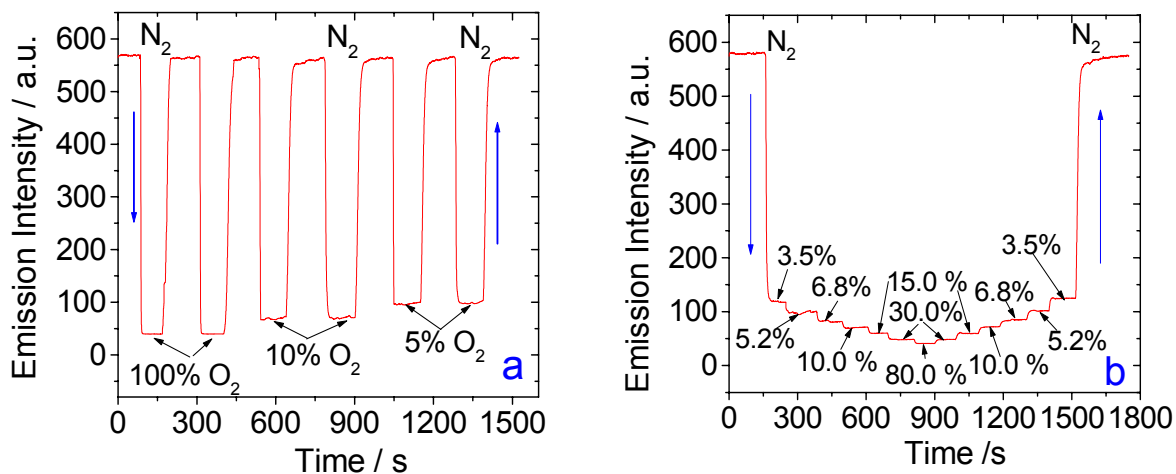


Figure S9. Phosphorescent intensity response of sensing films of the **Pt-1** in IMPEK-C to (a) O_2/N_2 saturation cycles and (b) dynamic response to variation of the oxygen partial pressures. λ_{ex} = 458 nm, λ_{em} = 630 nm. The numbers indicate the O_2 concentration in mixed O_2/N_2 gas (v/v). 25 °C.

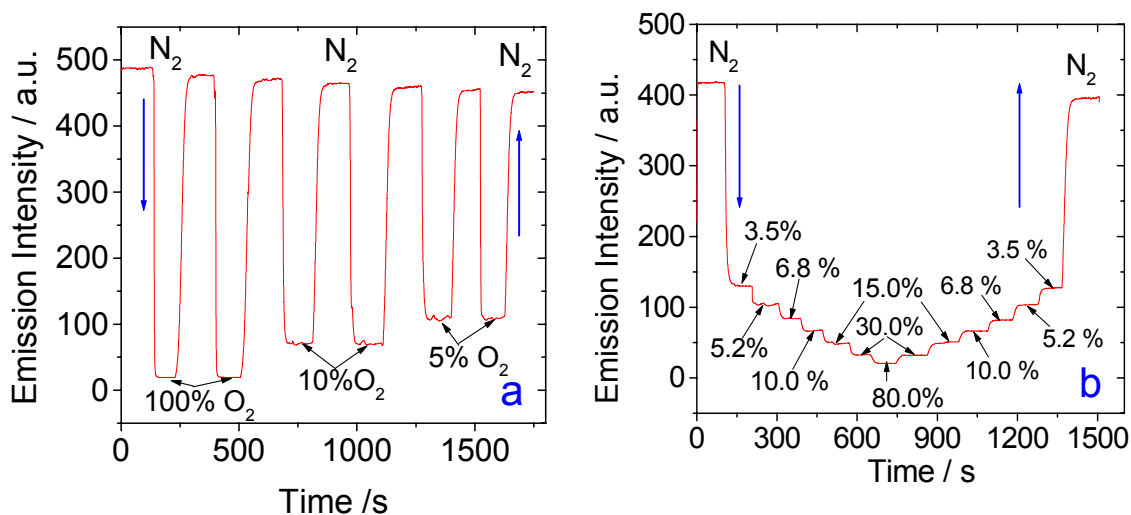
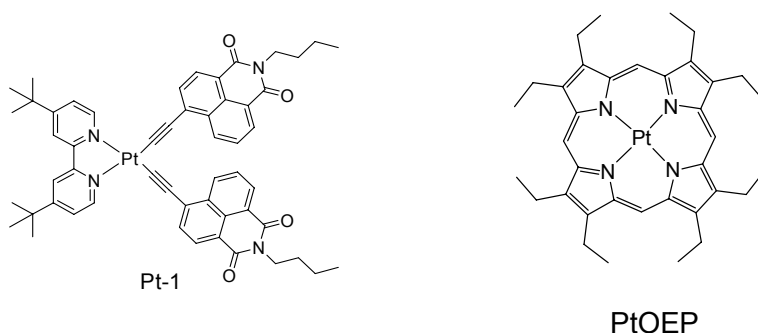


Figure S10. Phosphorescent intensity response of sensing films of the **PtOEP** in IMPEK-C to (a) O_2/N_2 saturation cycles and (b) dynamic response to variation of the oxygen partial pressures. λ_{ex} = 549 nm, λ_{em} = 648 nm. The numbers indicate the O_2 concentration in mixed O_2/N_2 gas (v/v). 25 °C.



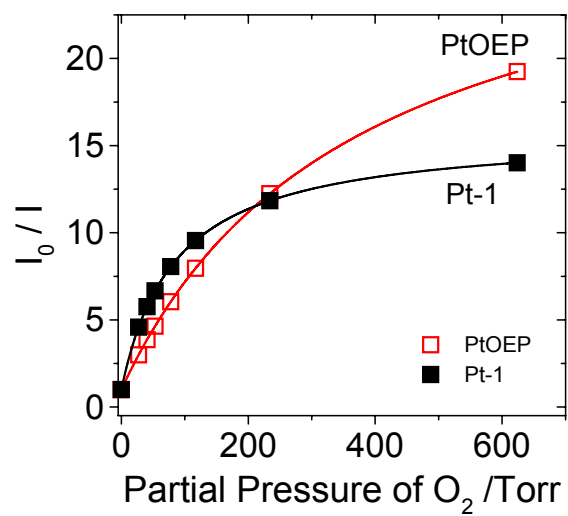


Figure S11. Two-sites model plots for sensing films of **Pt-1** and **PtOEP** in polymer IMPEK-C. The solid lines are the fitting results of the data with the two-site model.

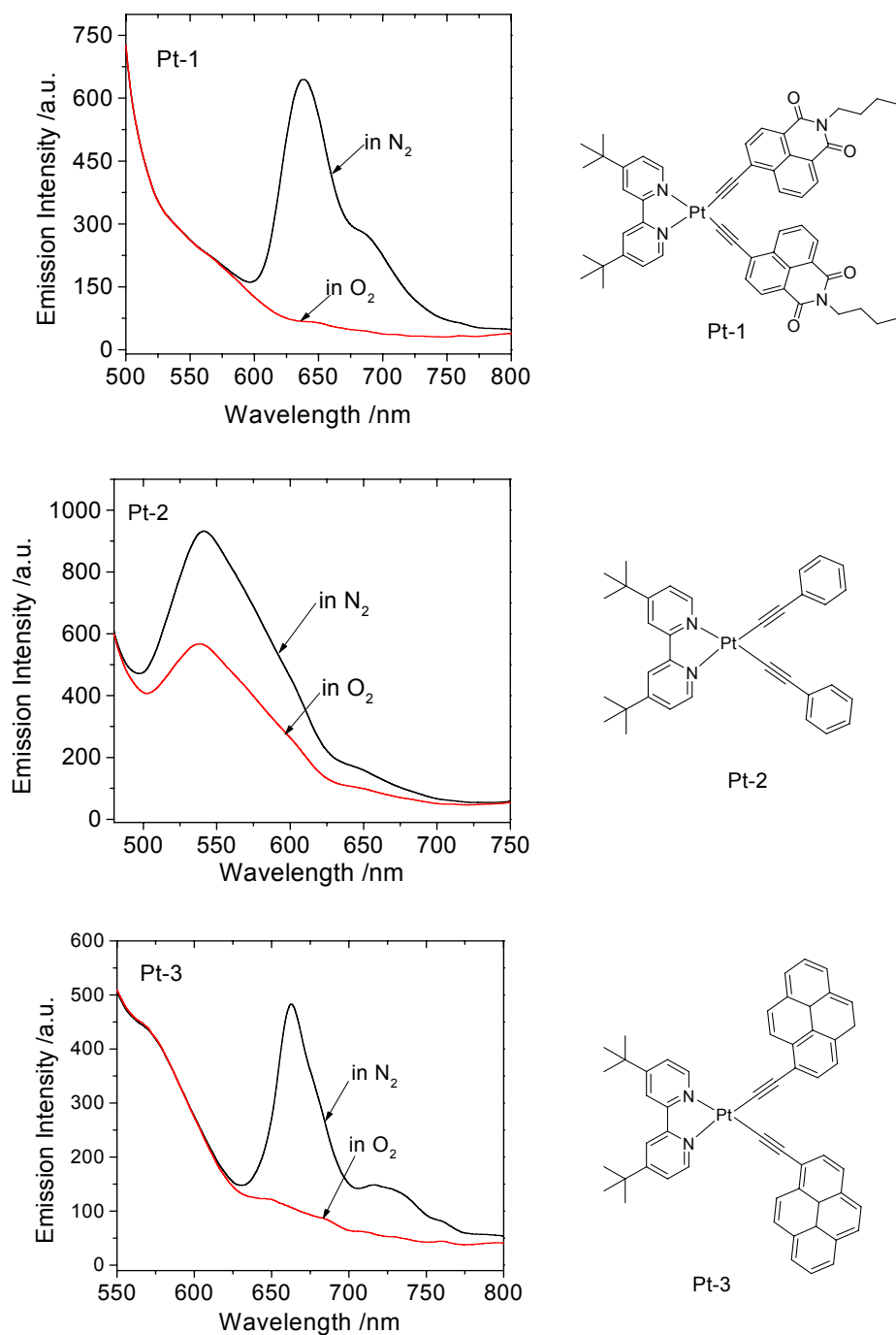


Figure S12. Emission spectra of complexes **Pt-1**, **Pt-2** and **Pt-3** in IMPEK-C films under N_2 and O_2 . For **Pt-1**, λ_{ex} = 458 nm; **Pt-2**, λ_{ex} = 430 nm; **Pt-3**, λ_{ex} = 468 nm.

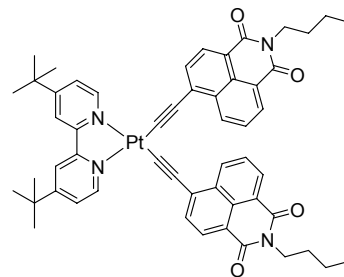
Pt-1

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

0 1

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	1	B4	2	A3	3	D2
C	4	B5	3	A4	2	D3
C	6	B6	4	A5	3	D4
C	7	B7	6	A6	4	D5
C	8	B8	7	A7	6	D6
C	9	B9	8	A8	7	D7
H	1	B10	5	A9	4	D8
H	5	B11	1	A10	2	D9
H	9	B12	8	A11	7	D10
H	10	B13	9	A12	8	D11
N	10	B14	9	A13	8	D12
N	5	B15	1	A14	2	D13
Pt	15	B16	10	A15	9	D14
C	17	B17	15	A16	10	D15
C	18	B18	17	A17	15	D16
C	17	B19	15	A18	10	D17
C	20	B20	17	A19	15	D18
H	7	B21	6	A20	4	D19
H	3	B22	2	A21	1	D20
C	8	B23	7	A22	6	D21
C	2	B24	1	A23	5	D22
C	24	B25	8	A24	7	D23
H	26	B26	24	A25	8	D24
H	26	B27	24	A26	8	D25
H	26	B28	24	A27	8	D26
C	24	B29	8	A28	7	D27
H	30	B30	24	A29	8	D28
H	30	B31	24	A30	8	D29
H	30	B32	24	A31	8	D30
C	24	B33	8	A32	7	D31
H	34	B34	24	A33	8	D32
H	34	B35	24	A34	8	D33
H	34	B36	24	A35	8	D34
C	25	B37	2	A36	1	D35
H	38	B38	25	A37	2	D36
H	38	B39	25	A38	2	D37
H	38	B40	25	A39	2	D38
C	25	B41	2	A40	1	D39



H	42	B42	25	A41	2	D40
H	42	B43	25	A42	2	D41
H	42	B44	25	A43	2	D42
C	25	B45	2	A44	1	D43
H	46	B46	25	A45	2	D44
H	46	B47	25	A46	2	D45
H	46	B48	25	A47	2	D46
C	19	B49	18	A48	17	D47
C	50	B50	19	A49	18	D48
C	50	B51	19	A50	18	D49
C	51	B52	50	A51	19	D50
C	51	B53	50	A52	19	D51
C	52	B54	50	A53	19	D52
H	52	B55	50	A54	19	D53
C	53	B56	51	A55	50	D54
H	53	B57	51	A56	50	D55
C	54	B58	51	A57	50	D56
C	55	B59	52	A58	50	D57
H	55	B60	52	A59	50	D58
C	59	B61	54	A60	51	D59
H	57	B62	53	A61	51	D60
H	62	B63	59	A62	54	D61
C	21	B64	20	A63	17	D62
C	65	B65	21	A64	20	D63
C	65	B66	21	A65	20	D64
C	66	B67	65	A66	21	D65
C	66	B68	65	A67	21	D66
C	67	B69	65	A68	21	D67
H	67	B70	65	A69	21	D68
C	68	B71	66	A70	65	D69
H	68	B72	66	A71	65	D70
C	69	B73	66	A72	65	D71
C	70	B74	67	A73	65	D72
H	70	B75	67	A74	65	D73
C	74	B76	69	A75	66	D74
H	72	B77	68	A76	66	D75
H	77	B78	74	A77	69	D76
C	59	B79	54	A78	51	D77
C	60	B80	55	A79	52	D78
N	80	B81	59	A80	54	D79
O	81	B82	60	A81	55	D80
O	80	B83	59	A82	54	D81
C	82	B84	80	A83	59	D82
H	85	B85	82	A84	80	D83
H	85	B86	82	A85	80	D84
H	85	B87	82	A86	80	D85
C	75	B88	70	A87	67	D86

C	74	B89	69	A88	66	D87
O	90	B90	74	A89	69	D88
O	89	B91	75	A90	70	D89
N	90	B92	74	A91	69	D90
C	93	B93	90	A92	74	D91
H	94	B94	93	A93	90	D92
H	94	B95	93	A94	90	D93
H	94	B96	93	A95	90	D94

B1	1.40467028
B2	1.40711925
B3	1.39614318
B4	1.39290986
B5	1.47544492
B6	1.39613282
B7	1.40711916
B8	1.40466962
B9	1.39291885
B10	1.08100187
B11	1.08209657
B12	1.08100412
B13	1.08209923
B14	1.35095501
B15	1.35094743
B16	2.10405258
B17	1.95869378
B18	1.23191165
B19	1.95869143
B20	1.23191060
B21	1.08204013
B22	1.08205064
B23	1.53903608
B24	1.53904308
B25	1.55450621
B26	1.09541337
B27	1.09575481
B28	1.09559837
B29	1.55453863
B30	1.09582923
B31	1.09540660
B32	1.09564551
B33	1.54549649
B34	1.09579138
B35	1.09581572
B36	1.09486646
B37	1.55450783
B38	1.09541136

B39	1.09575507
B40	1.09559844
B41	1.55453578
B42	1.09582220
B43	1.09540575
B44	1.09564573
B45	1.54548616
B46	1.09579107
B47	1.09581543
B48	1.09486742
B49	1.42017694
B50	1.44517382
B51	1.40171798
B52	1.41939800
B53	1.43063282
B54	1.40310981
B55	1.08370161
B56	1.38564022
B57	1.08475548
B58	1.42257066
B59	1.39073048
B60	1.08412741
B61	1.38819455
B62	1.08477025
B63	1.08409553
B64	1.42016127
B65	1.44517735
B66	1.40171711
B67	1.41939140
B68	1.43062828
B69	1.40311678
B70	1.08370000
B71	1.38563903
B72	1.08475511
B73	1.42256728
B74	1.39073844
B75	1.08412765
B76	1.38818944
B77	1.08477096
B78	1.08409507
B79	1.47606612
B80	1.47153495
B81	1.40342763
B82	1.25211759
B83	1.25205358
B84	1.47400548
B85	1.09261002

B86	1.09242054
B87	1.08753307
B88	1.47153613
B89	1.47607581
B90	1.25205825
B91	1.25211046
B92	1.40341126
B93	1.47400622
B94	1.09245179
B95	1.08753286
B96	1.09257842
A1	116.53995933
A2	121.31638778
A3	120.39907227
A4	124.32668920
A5	124.32598087
A6	121.31772108
A7	116.53936633
A8	120.39870341
A9	118.30267542
A10	122.36875824
A11	121.29911336
A12	122.36726703
A13	122.05626847
A14	122.05596743
A15	124.95372919
A16	96.15441326
A17	177.52945859
A18	174.08212368
A19	177.53749224
A20	119.20150031
A21	119.47998000
A22	120.23832651
A23	123.21950231
A24	109.24211602
A25	111.94235335
A26	109.73721622
A27	110.99574823
A28	109.18860856
A29	109.76068336
A30	111.91903099
A31	110.98805075
A32	111.97461819
A33	111.78659280
A34	111.79828079
A35	109.38195244
A36	109.23847185

A37	111.94142850
A38	109.73577752
A39	110.99434967
A40	109.19305155
A41	109.75819322
A42	111.92068986
A43	110.98873168
A44	111.97385903
A45	111.78705488
A46	111.79751137
A47	109.38423150
A48	179.54113739
A49	120.76601879
A50	120.63795225
A51	122.28397246
A52	119.16502355
A53	121.50107758
A54	118.68086991
A55	120.98162055
A56	118.23788054
A57	119.49008056
A58	120.94594882
A59	120.62601421
A60	120.39406575
A61	120.01897209
A62	118.52599882
A63	179.53517692
A64	120.75957502
A65	120.64538052
A66	122.28360822
A67	119.16626110
A68	121.50074806
A69	118.68153743
A70	120.98270011
A71	118.23827039
A72	119.49012869
A73	120.94677252
A74	120.62501641
A75	120.39486466
A76	120.01914016
A77	118.52562602
A78	120.08750723
A79	119.72675112
A80	117.33462253
A81	122.66286450
A82	122.85296963
A83	116.68834597

A84	109.85483900
A85	109.76994815
A86	107.63507486
A87	119.72703014
A88	120.08735933
A89	122.85173010
A90	122.66323713
A91	117.33515967
A92	116.68898156
A93	109.77827909
A94	107.63455778
A95	109.84584471
D1	0.00296279
D2	-0.02692931
D3	-179.92338158
D4	-0.28006141
D5	-179.91741008
D6	0.00340077
D7	-0.03159632
D8	-179.95810853
D9	179.98915018
D10	179.95391251
D11	179.99163407
D12	0.01087431
D13	0.00703173
D14	179.75610452
D15	0.36239893
D16	-0.31047422
D17	-178.33752257
D18	-1.36248724
D19	0.07846432
D20	-179.99265330
D21	-179.92973547
D22	179.91900258
D23	-59.58167452
D24	60.34224042
D25	179.93881322
D26	-60.52731540
D27	60.12026083
D28	-179.62160529
D29	-60.00771849
D30	60.84588479
D31	-179.75003499
D32	-61.12416251
D33	60.83835043
D34	179.86867112
D35	120.44914473

D36	60.29500316
D37	179.89318273
D38	-60.57405166
D39	-119.84888397
D40	-179.61688279
D41	-60.00399808
D42	60.85100340
D43	0.28420580
D44	-61.12805560
D45	60.83390097
D46	179.86136095
D47	-72.55514593
D48	143.85407049
D49	-35.56365842
D50	1.52907678
D51	-178.63834927
D52	178.87789810
D53	-1.08453683
D54	-179.79887837
D55	0.78031923
D56	179.61757055
D57	-0.09131350
D58	-179.96419927
D59	0.34251836
D60	-179.66234866
D61	179.81263380
D62	-64.48246348
D63	135.00253730
D64	-44.40410938
D65	1.55802348
D66	-178.61297348
D67	178.85423166
D68	-1.10234576
D69	-179.79809700
D70	0.78834608
D71	179.61392113
D72	-0.08914638
D73	-179.96027923
D74	0.34827070
D75	-179.66070361
D76	179.80786034
D77	-179.72945116
D78	-179.58318298
D79	-0.32622425
D80	0.32441185
D81	179.59225505
D82	-179.77595315

D83	-59.90378937
D84	58.93728119
D85	179.52360812
D86	-179.58032349
D87	-179.72551720
D88	179.60746988
D89	0.33241693
D90	-0.31932773
D91	-179.77908453
D92	59.16902298
D93	179.74352019
D94	-59.67259386

1 2 1.5 5 1.5 11 1.0
2 3 1.5 25 1.0
3 4 1.5 23 1.0
4 6 1.0 16 1.5
5 12 1.0 16 1.5
6 7 1.5 15 1.5
7 8 1.5 22 1.0
8 9 1.5 24 1.0
9 10 1.5 13 1.0
10 14 1.0 15 1.5
11
12
13
14
15 17 1.0
16 17 1.0
17 18 1.0 20 1.0
18 19 3.0
19 50 1.5
20 21 3.0
21 65 1.5
22
23
24 26 1.0 30 1.0 34 1.0
25 38 1.0 42 1.0 46 1.0
26 27 1.0 28 1.0 29 1.0
27
28
29
30 31 1.0 32 1.0 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0

35
36
37
38 39 1.0 40 1.0 41 1.0
39
40
41
42 43 1.0 44 1.0 45 1.0
43
44
45
46 47 1.0 48 1.0 49 1.0
47
48
49
50 51 1.5 52 1.5
51 53 1.5 54 1.5
52 55 1.5 56 1.0
53 57 2.0 58 1.0
54 59 1.5 60 1.5
55 60 1.5 61 1.0
56
57 62 1.5 63 1.0
58
59 62 2.0 80 1.0
60 81 1.0
61
62 64 1.0
63
64
65 66 1.5 67 1.5
66 68 1.5 69 1.5
67 70 1.5 71 1.0
68 72 2.0 73 1.0
69 74 1.5 75 1.5
70 75 1.5 76 1.0
71
72 77 1.5 78 1.0
73
74 77 2.0 90 1.0
75 89 1.0
76
77 79 1.0
78
79
80 82 1.0 84 2.0
81 82 1.0 83 2.0

82 85 1.0
 83
 84
 85 86 1.0 87 1.0 88 1.0
 86
 87
 88
 89 92 2.0 93 1.0
 90 91 2.0 93 1.0
 91
 92
 93 94 1.0
 94 95 1.0 96 1.0 97 1.0
 95
 96
 97

Pt-2

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

0 1

0 1

C

C

1

B1

C

2

B2

1

A1

C

3

B3

2

A2

1

D1

C

1

B4

2

A3

3

D2

C

4

B5

3

A4

2

D3

C

6

B6

4

A5

3

D4

C

7

B7

6

A6

4

D5

C

8

B8

7

A7

6

D6

C

9

B9

8

A8

7

D7

H

1

B10

5

A9

4

D8

H

5

B11

1

A10

2

D9

H

9

B12

8

A11

7

D10

H

10

B13

9

A12

8

D11

N

10

B14

9

A13

8

D12

N

5

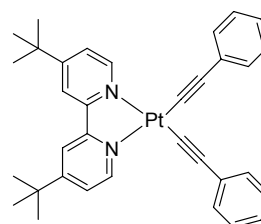
B15

1

A14

2

D13



Pt	16	B16	5	A15	1	D14
C	17	B17	16	A16	5	D15
C	18	B18	17	A17	16	D16
C	17	B19	16	A18	5	D17
C	20	B20	17	A19	16	D18
C	19	B21	18	A20	17	D19
C	22	B22	19	A21	18	D20
C	22	B23	19	A22	18	D21
C	23	B24	22	A23	19	D22
H	23	B25	22	A24	19	D23
C	24	B26	22	A25	19	D24
H	24	B27	22	A26	19	D25
C	27	B28	24	A27	22	D26
H	25	B29	23	A28	22	D27
H	27	B30	24	A29	22	D28
H	29	B31	27	A30	24	D29
C	21	B32	20	A31	17	D30
C	33	B33	21	A32	20	D31
C	33	B34	21	A33	20	D32
C	34	B35	33	A34	21	D33
H	34	B36	33	A35	21	D34
C	35	B37	33	A36	21	D35
H	35	B38	33	A37	21	D36
C	36	B39	34	A38	33	D37
H	36	B40	34	A39	33	D38
H	38	B41	35	A40	33	D39
H	40	B42	36	A41	34	D40
H	7	B43	6	A42	4	D41
H	3	B44	2	A43	1	D42
C	8	B45	7	A44	6	D43
C	2	B46	1	A45	5	D44
C	46	B47	8	A46	7	D45
H	48	B48	46	A47	8	D46
H	48	B49	46	A48	8	D47
H	48	B50	46	A49	8	D48
C	46	B51	8	A50	7	D49
H	52	B52	46	A51	8	D50
H	52	B53	46	A52	8	D51
H	52	B54	46	A53	8	D52
C	46	B55	8	A54	7	D53
H	56	B56	46	A55	8	D54
H	56	B57	46	A56	8	D55
H	56	B58	46	A57	8	D56
C	47	B59	2	A58	1	D57
H	60	B60	47	A59	2	D58
H	60	B61	47	A60	2	D59
H	60	B62	47	A61	2	D60

C	47	B63	2	A62	1	D61
H	64	B64	47	A63	2	D62
H	64	B65	47	A64	2	D63
H	64	B66	47	A65	2	D64
C	47	B67	2	A66	1	D65
H	68	B68	47	A67	2	D66
H	68	B69	47	A68	2	D67
H	68	B70	47	A69	2	D68

B1	1.40052013
B2	1.40232034
B3	1.39449600
B4	1.39067089
B5	1.48070172
B6	1.39449593
B7	1.40232078
B8	1.40051974
B9	1.39067154
B10	1.08284495
B11	1.08526781
B12	1.08284488
B13	1.08526796
B14	1.34083336
B15	1.34083478
B16	2.12048940
B17	1.95129109
B18	1.22526400
B19	1.95129066
B20	1.22526371
B21	1.42605192
B22	1.41193856
B23	1.41102065
B24	1.39243175
B25	1.08568741
B26	1.39290554
B27	1.08653294
B28	1.39720452
B29	1.08728740
B30	1.08744563
B31	1.08682719
B32	1.42605164
B33	1.41102066
B34	1.41193824
B35	1.39290576
B36	1.08653289
B37	1.39243153
B38	1.08568754

B39	1.39720440
B40	1.08744562
B41	1.08728743
B42	1.08682717
B43	1.08312679
B44	1.08312674
B45	1.53590715
B46	1.53590699
B47	1.54787861
B48	1.09531916
B49	1.09611789
B50	1.09564522
B51	1.54787786
B52	1.09611739
B53	1.09531924
B54	1.09564508
B55	1.54057245
B56	1.09585049
B57	1.09585031
B58	1.09520861
B59	1.54787720
B60	1.09531923
B61	1.09611789
B62	1.09564545
B63	1.54787920
B64	1.09611735
B65	1.09531924
B66	1.09564480
B67	1.54057252
B68	1.09585038
B69	1.09585042
B70	1.09520857
A1	116.20245011
A2	121.36316974
A3	120.26882263
A4	123.88226872
A5	123.88227494
A6	121.36318408
A7	116.20244685
A8	120.26879318
A9	118.25601795
A10	122.52062137
A11	121.47521237
A12	122.52057264
A13	122.52366124
A14	122.52363843
A15	125.13488308

A16	173.67646105
A17	177.02831061
A18	96.35837604
A19	177.03066668
A20	177.69744622
A21	120.53441242
A22	121.50019225
A23	120.83780711
A24	118.65681350
A25	120.94745912
A26	118.91920331
A27	120.37403833
A28	119.53804026
A29	119.61549950
A30	120.28645384
A31	177.69792235
A32	121.50024406
A33	120.53438414
A34	120.94747289
A35	118.91920595
A36	120.83781275
A37	118.65686021
A38	120.37404588
A39	119.61540369
A40	119.53805478
A41	120.28659152
A42	119.10674198
A43	119.53010936
A44	120.36554417
A45	123.43200912
A46	109.19667547
A47	112.04881929
A48	109.98530194
A49	111.11341773
A50	109.19697175
A51	109.98509593
A52	112.04901057
A53	111.11344438
A54	112.06215008
A55	111.94107614
A56	111.94094556
A57	109.47360590
A58	109.19692007
A59	112.04899211
A60	109.98530425
A61	111.11343618
A62	109.19670017

A63	109.98510462
A64	112.04883165
A65	111.11344943
A66	112.06213479
A67	111.94116011
A68	111.94086293
A69	109.47359773
D1	0.00000000
D2	0.00000000
D3	-180.00000000
D4	0.01227788
D5	-180.00000000
D6	0.00000000
D7	0.00000000
D8	-180.00000000
D9	-180.00000000
D10	-180.00000000
D11	-180.00000000
D12	0.00000000
D13	0.00000000
D14	-179.99238172
D15	179.98609243
D16	0.08581886
D17	-0.00614946
D18	0.21181860
D19	179.92307105
D20	-0.01759053
D21	179.98238279
D22	180.00000000
D23	0.00000000
D24	-180.00000000
D25	0.00000000
D26	0.00000000
D27	-180.00000000
D28	180.00000000
D29	180.00000000
D30	-179.95628469
D31	179.72445947
D32	-0.27493292
D33	-180.00000000
D34	0.00000000
D35	180.00000000
D36	0.00000000
D37	0.00000000
D38	180.00000000
D39	-180.00000000
D40	180.00000000

D41	0.00000000
D42	180.00000000
D43	180.00000000
D44	180.00000000
D45	-59.87294535
D46	60.27363002
D47	179.92540575
D48	-60.46354574
D49	59.86871522
D50	-179.92624106
D51	-60.27458328
D52	60.46276519
D53	180.00000000
D54	-60.94818908
D55	60.94778631
D56	180.00000000
D57	120.12921223
D58	60.27264291
D59	179.92441131
D60	-60.46460523
D61	-120.12912178
D62	-179.92697695
D63	-60.27533796
D64	60.46194755
D65	0.00000000
D66	-60.94874212
D67	60.94722820
D68	180.00000000

1 2 1.5 5 1.5 11 1.0
2 3 1.5 47 1.0
3 4 1.5 45 1.0
4 6 1.0 16 1.5
5 12 1.0 16 1.5
6 7 1.5 15 1.5
7 8 1.5 44 1.0
8 9 1.5 46 1.0
9 10 1.5 13 1.0
10 14 1.0 15 1.5
11
12
13
14
15 17 1.0
16 17 1.0
17 18 1.0 20 1.0
18 19 3.0

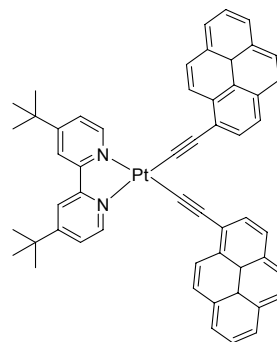
19 22 1.0
20 21 3.0
21 33 1.0
22 23 1.5 24 1.5
23 25 1.5 26 1.0
24 27 1.5 28 1.0
25 29 1.5 30 1.0
26
27 29 1.5 31 1.0
28
29 32 1.0
30
31
32
33 34 1.5 35 1.5
34 36 1.5 37 1.0
35 38 1.5 39 1.0
36 40 1.5 41 1.0
37
38 40 1.5 42 1.0
39
40 43 1.0
41
42
43
44
45
46 48 1.0 52 1.0 56 1.0
47 60 1.0 64 1.0 68 1.0
48 49 1.0 50 1.0 51 1.0
49
50
51
52 53 1.0 54 1.0 55 1.0
53
54
55
56 57 1.0 58 1.0 59 1.0
57
58
59
60 61 1.0 62 1.0 63 1.0
61
62
63
64 65 1.0 66 1.0 67 1.0
65

66
 67
 68 69 1.0 70 1.0 71 1.0
 69
 70
 71

Pt-3

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



Pt-3

0 1						
C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	1	B4	2	A3	3	D2
C	4	B5	3	A4	2	D3
C	6	B6	4	A5	3	D4
C	7	B7	6	A6	4	D5
C	8	B8	7	A7	6	D6
C	9	B9	8	A8	7	D7
H	1	B10	5	A9	4	D8
H	5	B11	1	A10	2	D9
H	9	B12	8	A11	7	D10
H	10	B13	9	A12	8	D11
N	10	B14	9	A13	8	D12
N	5	B15	1	A14	2	D13
Pt	16	B16	5	A15	1	D14
C	17	B17	16	A16	5	D15
C	18	B18	17	A17	16	D16
C	17	B19	16	A18	5	D17
C	20	B20	17	A19	16	D18
H	7	B21	6	A20	4	D19
H	3	B22	2	A21	1	D20
C	8	B23	7	A22	6	D21
C	2	B24	1	A23	5	D22
C	24	B25	8	A24	7	D23

H	26	B26	24	A25	8	D24
H	26	B27	24	A26	8	D25
H	26	B28	24	A27	8	D26
C	24	B29	8	A28	7	D27
H	30	B30	24	A29	8	D28
H	30	B31	24	A30	8	D29
H	30	B32	24	A31	8	D30
C	24	B33	8	A32	7	D31
H	34	B34	24	A33	8	D32
H	34	B35	24	A34	8	D33
H	34	B36	24	A35	8	D34
C	25	B37	2	A36	1	D35
H	38	B38	25	A37	2	D36
H	38	B39	25	A38	2	D37
H	38	B40	25	A39	2	D38
C	25	B41	2	A40	1	D39
H	42	B42	25	A41	2	D40
H	42	B43	25	A42	2	D41
H	42	B44	25	A43	2	D42
C	25	B45	2	A44	1	D43
H	46	B46	25	A45	2	D44
H	46	B47	25	A46	2	D45
H	46	B48	25	A47	2	D46
C	19	B49	18	A48	17	D47
C	50	B50	19	A49	18	D48
C	50	B51	19	A50	18	D49
C	51	B52	50	A51	19	D50
H	51	B53	50	A52	19	D51
C	52	B54	50	A53	19	D52
C	52	B55	50	A54	19	D53
C	53	B56	51	A55	50	D54
H	53	B57	51	A56	50	D55
C	55	B58	52	A57	50	D56
C	56	B59	52	A58	50	D57
H	56	B60	52	A59	50	D58
C	57	B61	53	A60	51	D59
C	59	B62	55	A61	52	D60
C	59	B63	55	A62	52	D61
H	60	B64	56	A63	52	D62
C	62	B65	57	A64	53	D63
H	62	B66	57	A65	53	D64
C	63	B67	59	A66	55	D65
C	64	B68	59	A67	55	D66
H	66	B69	62	A68	57	D67
C	69	B70	64	A69	59	D68
H	68	B71	63	A70	59	D69
H	69	B72	64	A71	59	D70

H	71	B73	69	A72	64	D71
C	21	B74	20	A73	17	D72
C	75	B75	21	A74	20	D73
C	75	B76	21	A75	20	D74
C	76	B77	75	A76	21	D75
H	76	B78	75	A77	21	D76
C	77	B79	75	A78	21	D77
C	77	B80	75	A79	21	D78
C	78	B81	76	A80	75	D79
H	78	B82	76	A81	75	D80
C	80	B83	77	A82	75	D81
C	81	B84	77	A83	75	D82
H	81	B85	77	A84	75	D83
C	82	B86	78	A85	76	D84
C	84	B87	80	A86	77	D85
C	84	B88	80	A87	77	D86
H	85	B89	81	A88	77	D87
C	87	B90	82	A89	78	D88
H	87	B91	82	A90	78	D89
C	88	B92	84	A91	80	D90
C	89	B93	84	A92	80	D91
H	91	B94	87	A93	82	D92
C	94	B95	89	A94	84	D93
H	93	B96	88	A95	84	D94
H	94	B97	89	A96	84	D95
H	96	B98	94	A97	89	D96

B1	1.40010243
B2	1.40284363
B3	1.39435531
B4	1.39076741
B5	1.48160180
B6	1.39435578
B7	1.40284296
B8	1.40010247
B9	1.39076741
B10	1.08282264
B11	1.08510340
B12	1.08282254
B13	1.08510324
B14	1.34101780
B15	1.34101829
B16	2.12084038
B17	1.95130796
B18	1.22599318
B19	1.95130805
B20	1.22599309

B21	1.08309322
B22	1.08309280
B23	1.53574828
B24	1.53574865
B25	1.54795088
B26	1.09533995
B27	1.09606167
B28	1.09567040
B29	1.54805644
B30	1.09600098
B31	1.09534645
B32	1.09567685
B33	1.54038955
B34	1.09576415
B35	1.09578769
B36	1.09514717
B37	1.54795063
B38	1.09534012
B39	1.09606198
B40	1.09567028
B41	1.54805571
B42	1.09600105
B43	1.09534637
B44	1.09567683
B45	1.54039063
B46	1.09576428
B47	1.09578765
B48	1.09514696
B49	1.42284085
B50	1.41078572
B51	1.42480871
B52	1.38689302
B53	1.08544680
B54	1.42764057
B55	1.43499407
B56	1.40579687
B57	1.08763764
B58	1.42921041
B59	1.36313760
B60	1.08586779
B61	1.43457369
B62	1.43005760
B63	1.42891336
B64	1.08786451
B65	1.36294268
B66	1.08769468
B67	1.40509456

B68	1.40535705
B69	1.08750678
B70	1.39376177
B71	1.08748410
B72	1.08755586
B73	1.08696221
B74	1.42284289
B75	1.41078416
B76	1.42480942
B77	1.38689394
B78	1.08544688
B79	1.42764077
B80	1.43499478
B81	1.40579590
B82	1.08763767
B83	1.42921103
B84	1.36313738
B85	1.08586762
B86	1.43457447
B87	1.43005733
B88	1.42891282
B89	1.08786449
B90	1.36294206
B91	1.08769468
B92	1.40509432
B93	1.40535706
B94	1.08750678
B95	1.39376163
B96	1.08748407
B97	1.08755584
B98	1.08696219
A1	116.20609601
A2	121.37185804
A3	120.26119517
A4	123.89192298
A5	123.89192782
A6	121.37180800
A7	116.20614249
A8	120.26118889
A9	118.16941968
A10	122.25223301
A11	121.56934070
A12	122.25216502
A13	122.53158478
A14	122.53161892
A15	125.15066875
A16	173.42792205

A17	176.38753221
A18	96.11310330
A19	176.38501092
A20	119.12849852
A21	119.49956569
A22	120.37742973
A23	123.41660231
A24	109.20963460
A25	112.07608485
A26	109.95335316
A27	111.13670869
A28	109.15795573
A29	109.94797781
A30	112.04840069
A31	111.12644440
A32	112.02267570
A33	111.92201194
A34	111.90530556
A35	109.54759459
A36	109.20951389
A37	112.07603962
A38	109.95346152
A39	111.13668866
A40	109.15818821
A41	109.94801953
A42	112.04848805
A43	111.12638931
A44	112.02272232
A45	111.92202005
A46	111.90522915
A47	109.54755602
A48	178.78187255
A49	119.76520969
A50	121.50962523
A51	121.56296949
A52	118.27248152
A53	119.62046293
A54	121.92353378
A55	121.16470453
A56	119.73603794
A57	120.05876038
A58	121.52175443
A59	117.70058434
A60	122.43671038
A61	120.17436253
A62	120.15630738
A63	120.27558154

A64	121.41471176
A65	118.22574458
A66	119.08502011
A67	119.15960380
A68	120.45563628
A69	120.75904004
A70	119.06635132
A71	119.08944220
A72	119.75783861
A73	178.78498942
A74	119.76513708
A75	121.50961437
A76	121.56297964
A77	118.27262893
A78	119.62034619
A79	121.92361339
A80	121.16467098
A81	119.73596662
A82	120.05874200
A83	121.52168685
A84	117.70056891
A85	122.43666907
A86	120.17435602
A87	120.15628207
A88	120.27561027
A89	121.41470134
A90	118.22564463
A91	119.08502083
A92	119.15958923
A93	120.45571003
A94	120.75903152
A95	119.06637086
A96	119.08948744
A97	119.75779056
D1	0.00000000
D2	0.08495162
D3	-179.88363265
D4	-1.54445454
D5	-179.88446846
D6	0.00000000
D7	0.08545757
D8	-179.97182041
D9	179.74941354
D10	179.96484374
D11	179.74971991
D12	-0.12354216
D13	-0.12317090

D14	178.90716576
D15	-173.08547535
D16	-0.70961382
D17	1.48728803
D18	5.18335309
D19	0.00924980
D20	-179.89446041
D21	180.00000000
D22	-179.91417760
D23	-59.64153559
D24	60.18632489
D25	179.80898157
D26	-60.59703467
D27	60.07490863
D28	-179.83019456
D29	-60.19902407
D30	60.57801268
D31	-179.78407703
D32	-61.00706387
D33	60.84348586
D34	179.89872563
D35	120.35901601
D36	60.18742892
D37	179.81009600
D38	-60.59593185
D39	-119.92443398
D40	-179.83077904
D41	-60.19962282
D42	60.57746786
D43	0.21662583
D44	-61.00832257
D45	60.84218117
D46	179.89745955
D47	-112.60403401
D48	-19.19529236
D49	160.27667760
D50	178.91373810
D51	-0.97775161
D52	-178.66485091
D53	1.55018298
D54	-0.03279745
D55	-179.93068752
D56	179.47170785
D57	-179.53105952
D58	1.35434541
D59	-179.64608348
D60	-179.80122817

D61	0.24805649
D62	-179.63106200
D63	179.95165173
D64	-0.04450600
D65	179.89951560
D66	-179.94096490
D67	-179.97181384
D68	-0.01021043
D69	-179.97616301
D70	-179.85738250
D71	-179.95126180
D72	-112.70750190
D73	-18.96914234
D74	160.50253310
D75	178.91425781
D76	-0.97736779
D77	-178.66530611
D78	1.54944089
D79	-0.03308133
D80	-179.93076472
D81	179.47180417
D82	-179.53102595
D83	1.35425317
D84	-179.64626676
D85	-179.80135307
D86	0.24784869
D87	-179.63118840
D88	179.95134689
D89	-0.04475472
D90	179.89947339
D91	-179.94095254
D92	-179.97189169
D93	-0.01015718
D94	-179.97616788
D95	-179.85727983
D96	-179.95125648

1 2 1.5 5 1.5 11 1.0
2 3 1.5 25 1.0
3 4 1.5 23 1.0
4 6 1.0 16 1.5
5 12 1.0 16 1.5
6 7 1.5 15 1.5
7 8 1.5 22 1.0
8 9 1.5 24 1.0
9 10 1.5 13 1.0
10 14 1.0 15 1.5

11
12
13
14
15 17 1.0
16 17 1.0
17 18 1.0 20 1.0
18 19 3.0
19 50 1.0
20 21 3.0
21 75 1.0
22
23
24 26 1.0 30 1.0 34 1.0
25 38 1.0 42 1.0 46 1.0
26 27 1.0 28 1.0 29 1.0
27
28
29
30 31 1.0 32 1.0 33 1.0
31
32
33
34 35 1.0 36 1.0 37 1.0
35
36
37
38 39 1.0 40 1.0 41 1.0
39
40
41
42 43 1.0 44 1.0 45 1.0
43
44
45
46 47 1.0 48 1.0 49 1.0
47
48
49
50 51 1.5 52 1.5
51 53 1.5 54 1.0
52 55 1.5 56 1.5
53 57 1.5 58 1.0
54
55 59 1.5 57 1.5
56 60 2.0 61 1.0
57 62 1.5

58
59 63 1.5 64 1.5
60 64 1.5 65 1.0
61
62 66 2.0 67 1.0
63 68 1.5 66 1.5
64 69 1.5
65
66 70 1.0
67
68 71 1.5 72 1.0
69 71 1.5 73 1.0
70
71 74 1.0
72
73
74
75 76 1.5 77 1.5
76 78 1.5 79 1.0
77 80 1.5 81 1.5
78 82 1.5 83 1.0
79
80 84 1.5 82 1.5
81 85 2.0 86 1.0
82 87 1.5
83
84 88 1.5 89 1.5
85 89 1.5 90 1.0
86
87 91 2.0 92 1.0
88 93 1.5 91 1.5
89 94 1.5
90
91 95 1.0
92
93 96 1.5 97 1.0
94 96 1.5 98 1.0
95
96 99 1.0
97
98
99