Bis[alkynylplatinum(II)] Terpyridine Molecular Tweezer with Conformationally-Rigid Spacer: Modulating the Binding Selectivity in a Three-Component Supramolecular Recognition System

Zijian Li, Yifei Han, Fan Jin, Zongchun Gao, Zhao Gao, Lei Ao, and Feng Wang*

CAS Key Laboratory of Soft Matter Chemistry,
iChEM (Collaborative Innovation Center of Chemistry for Energy Materials),
Department of Polymer Science and Engineering,
University of Science and Technology of China,
Hefei, Anhui 230026 P. R. China.
E-mail: drfwang@ustc.edu.cn.

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*1. ^{1}H NMR measurements for complex **2/3***

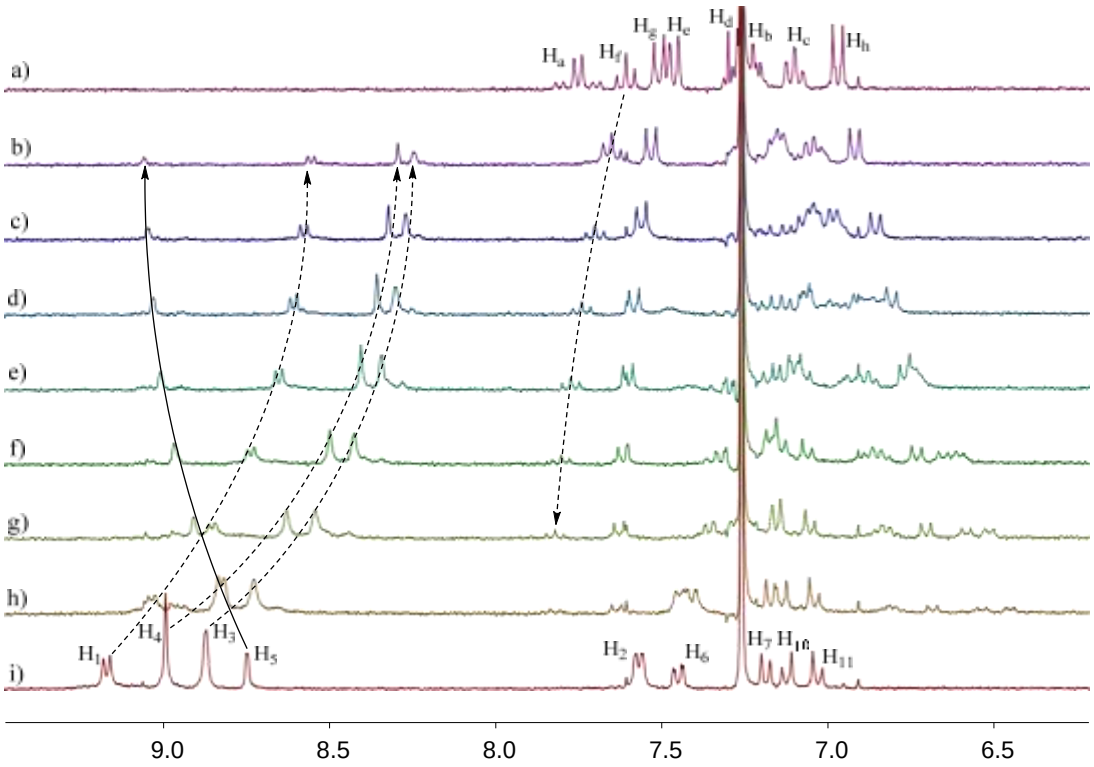

Figure S1. Partial ^{1}H NMR spectra (300 MHz, $CDCl_3$, room temperature) for complex **2/3** with different molar ratio : a) 0 : 6; b) 1 : 5; c) 2 : 4; d) 2.5 : 3.5; e) 3 : 3; f) 3.5 : 2.5; g) 4 : 2; h) 1 : 5; i) 6 : 0. $[\mathbf{2}]_0$ and $[\mathbf{3}]_0$ are the initial concentrations of **2** and **3**. $[\mathbf{2}]_0 + [\mathbf{3}]_0 = 2.00$ mM. The terpyridine protons $H_{1\text{-}4}$ on **2** undergo remarkable upfield shifts, whilst obvious downfield shifts are observed for proton H_f on **3**, as well as proton H_5 locating in the inner cavity of **2**.

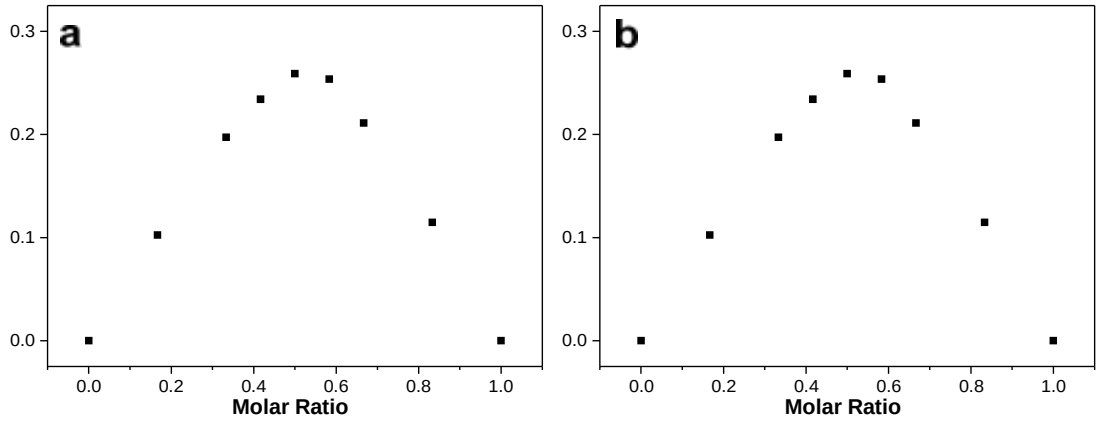

Figure S2. Job's plot for complex **2**/**3** based on the above ^{1}H NMR measurements (Figure S1), by probing the chemical shift changes of protons: a) H_3, and b) H_5. Both results demonstrate 1 : 1 binding stoichiometry between **2** and **3**.

2. ^{1}H-^{1}H *COSY NMR measurement for complex* ***2/3***

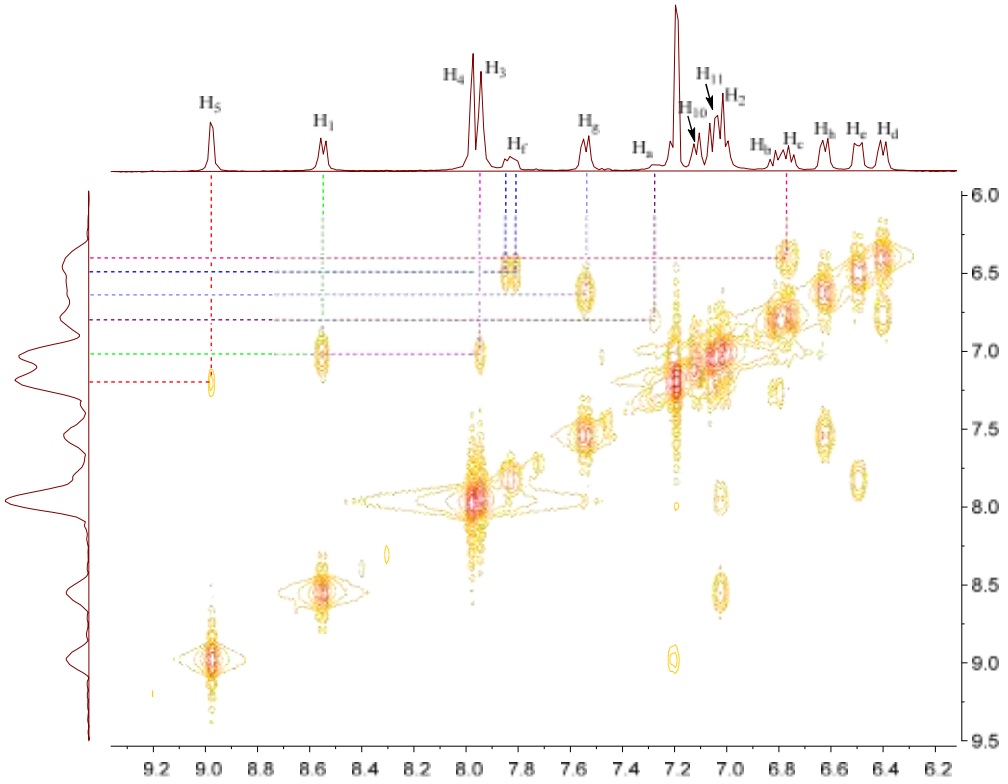

Figure S3. ^{1}H-^{1}H COSY NMR spectrum (400 MHz, $CDCl_3$, room temperature) of complex **2/3** (concentration: 2 mM for each compound). Strong correlations can be seen between proton H_1 and the neighboring proton H_2 on the terpyridine unit. Moreover, the correlations between H_e and the neighbouring proton H_f, H_b/H_c and H_d, H_g and H_h can also be observed. All of the correlation signals benefit for the accurate proton assignments.

3. UV-Vis molar ratio plot for complex ***2/3***

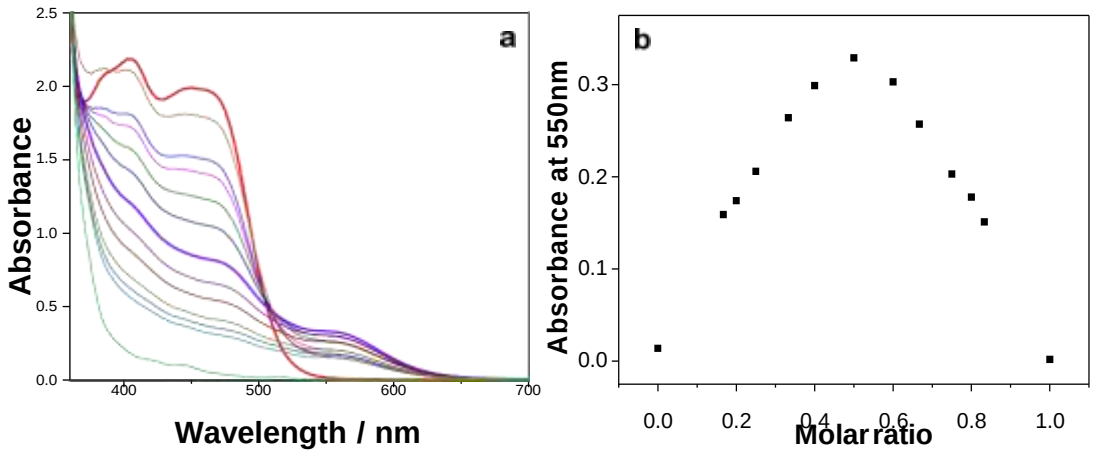

Figure S4. a) UV/Vis molar ratio plot for tweezer **2** and guest **3**. b) Job's plot curve showing 1 : 1 binding stoichiometry between **2** and **3**, by plotting the absorbance at 550 nm against the mole fraction of the guest.

*4. UV/Vis and fluorescent titrations for complex **2/3***

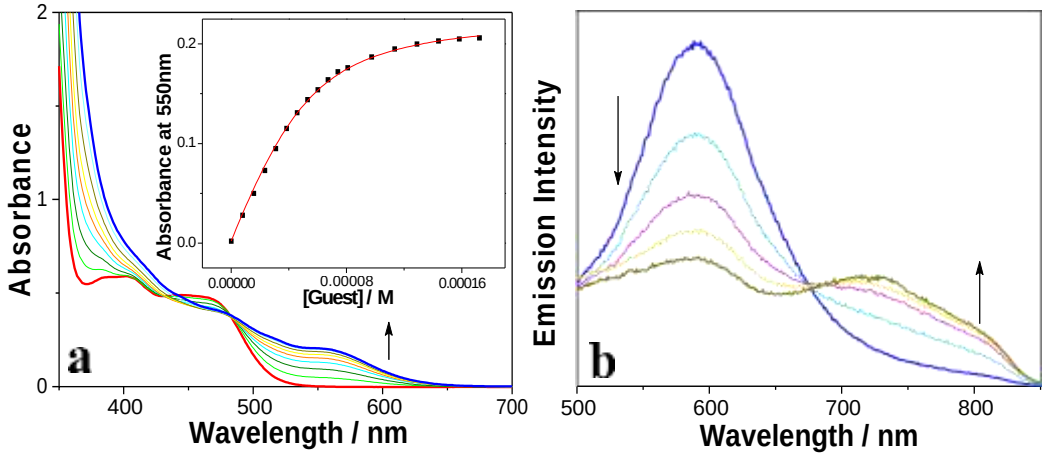

Figure S5. a) UV-Vis absorption spectral and b) emission spectral changes of **2** (chloroform, 0.05 mM, excitation at 460 nm) by gradual titration of **3** (1.00 mM). K_a for complex **2**/**3** is determined to be (7.00 ± 0.75) × 10^4 M^{-1}, by fitting the collected absorbance data at 550 nm with 1 : 1 model.

*5. UV/Vis and fluorescent titrations for complex **1/3***

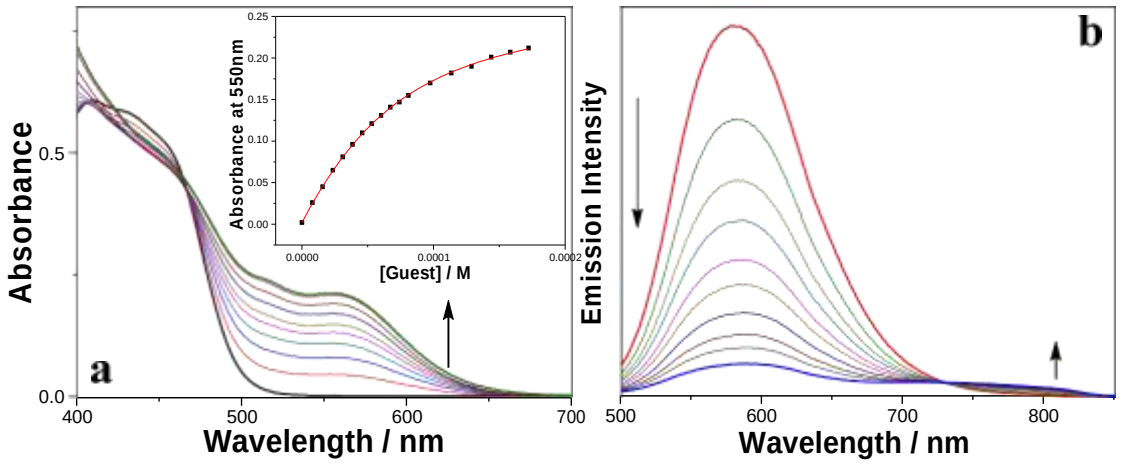

Figure S6. a) UV-Vis absorption and b) fluorescent changes of **1** (chloroform, 0.05 mM) upon gradual titration of **3** (1.00 mM). K_a for complex **1**/**3** is determined to be (2.45 ± 0.06) × 10^4 M^{-1}, by fitting the collected absorbance data at 550 nm with 1: 1 model.

*6. ITC measurements for complexes **1/3** and **2/3***

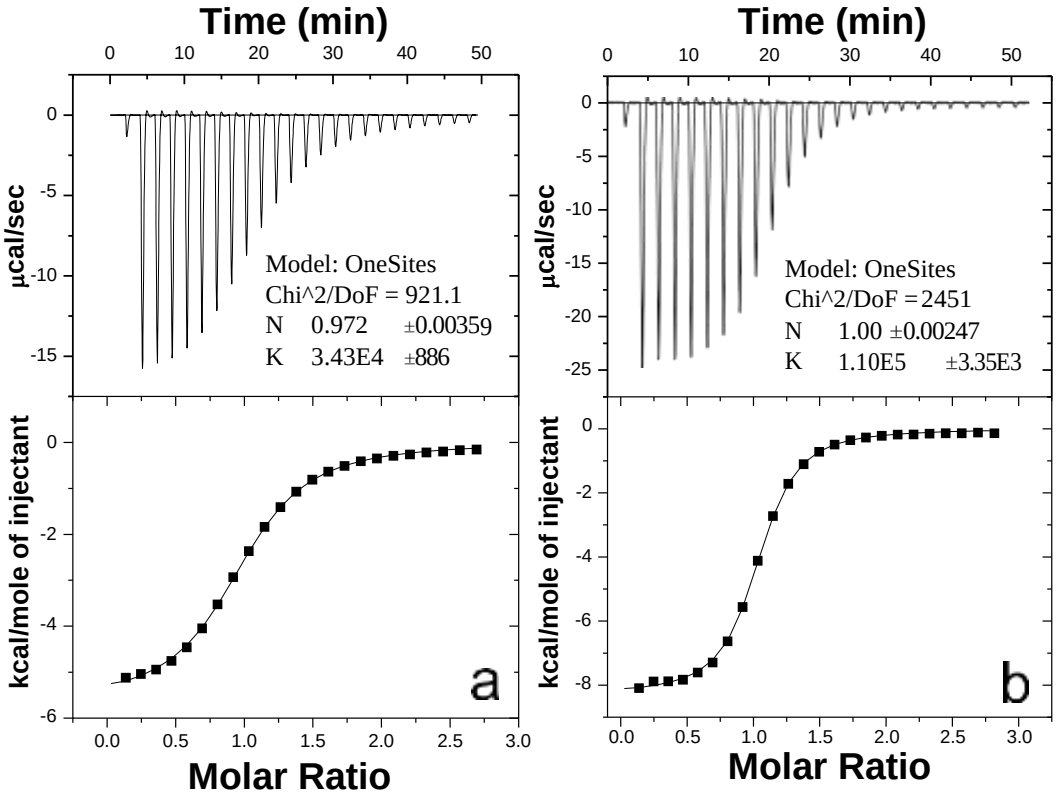

Figure S7. ITC data for titration of **3** (4.00 mM in chloroform) into the chloroform solution of a) **1** (0.20 mM) and b) **2** (0.20 mM).

*7. ^{1}H NMR measurements for complex **2/4***

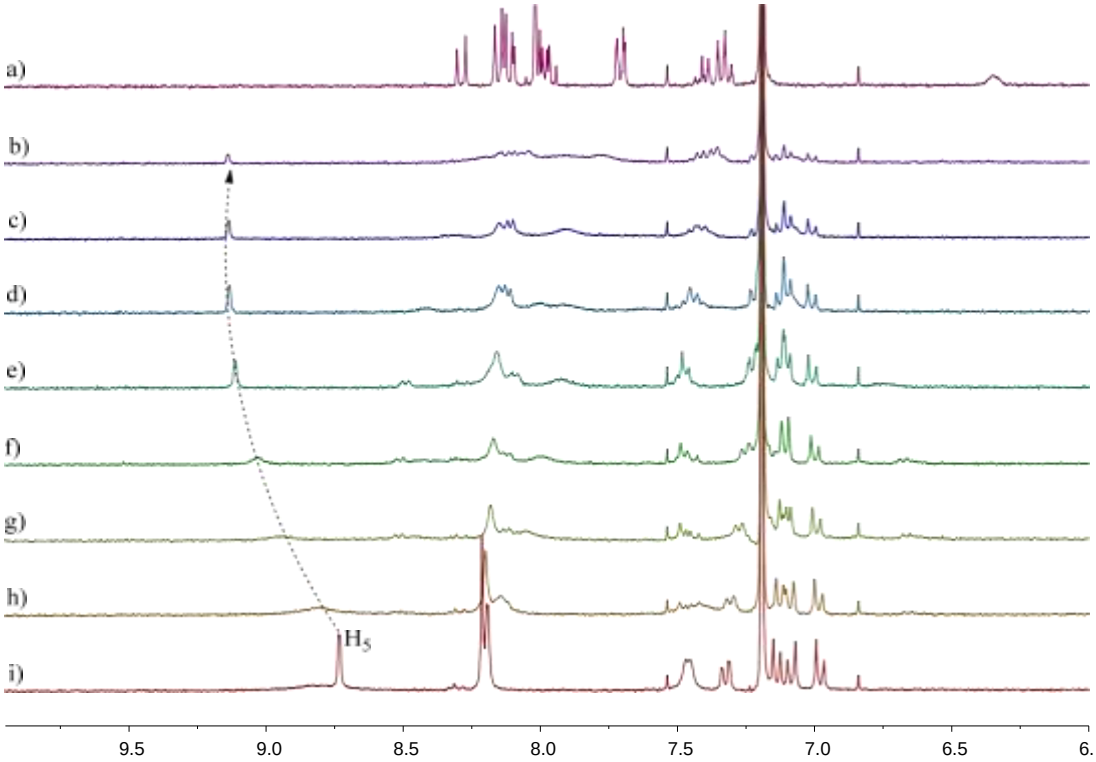

Figure S8. Partial 1H NMR spectra (300 MHz, CDCl3, room temperature) for the complex **2**/**4** with different molar ratio : a) 0 : 6; b) 1 : 5; c) 2 : 4; d) 2.5 : 3.5; e) 3 : 3; f) 3.5 : 2.5; g) 4 : 2; h) 1 : 5; i) 6 : 0. $[\mathbf{2}]_0$ and $[\mathbf{4}]_0$ are the initial concentrations of **2** and **4**. $[\mathbf{2}]_0 + [\mathbf{4}]_0 = 2.00$ mM.

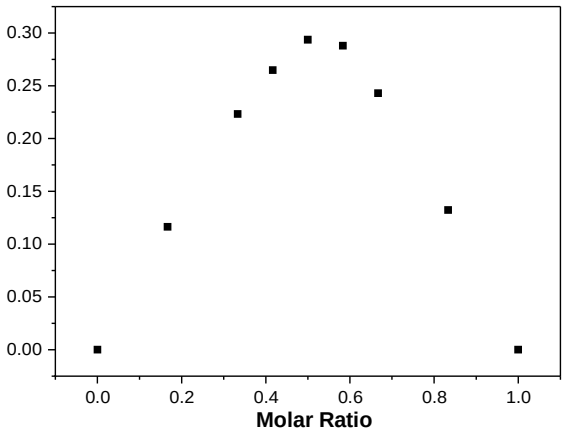

Figure S9. Job plot for complex **2**/**4** based on the above ^{1}H NMR measurements, probing the chemical shift changes for proton H_5. It shows 1 : 1 binding stoichiometry between **2** and **4**.

*8. UV/Vis titrations for complex **1/4***

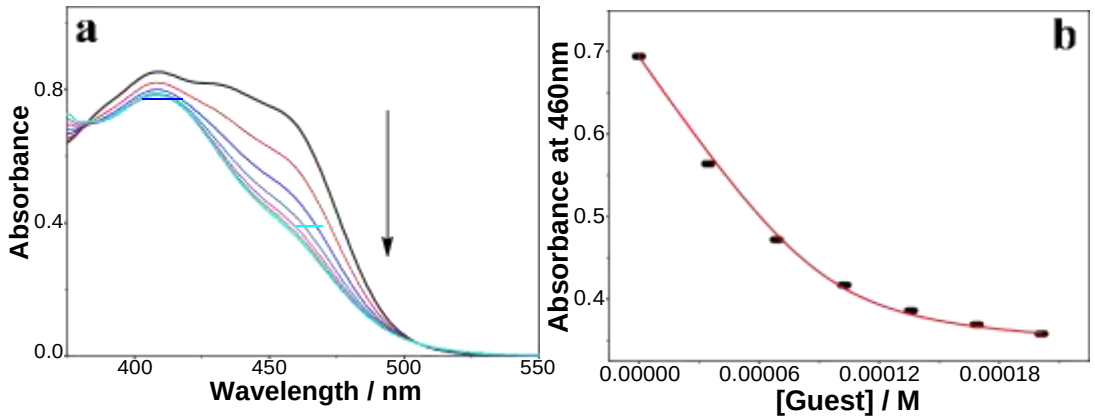

Figure S10. a) UV/Vis absorption spectral changes of **1** upon grudual addition of **4**; b) the intensity changes of absorbance at 460 nm upon addition of **4**. The MLCT (metal–to–ligand charge transfer) and LLCT (ligand–to–ligand charge transfer) bands of **1**, predominately locating on the region of approximately 400–500 nm, undergo gradual decrease for the absorption intensity upon progressive addition of **4**. Nonlinear curve-fitting of the collected absorbance data at 460 nm provides the K_a value of (1.31 ± 0.35) × 10^5 M^{-1}.

9.** UV/Vis and fluorescent titrations for complex **2/4

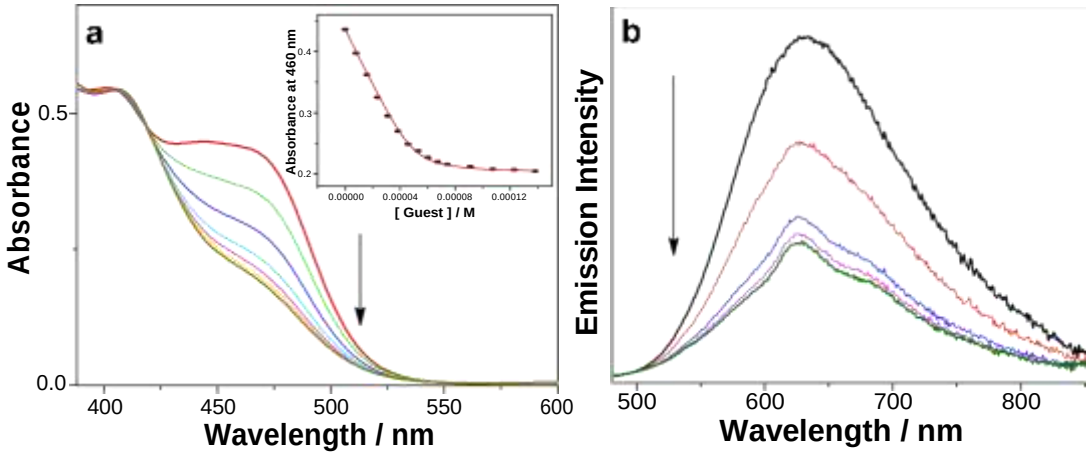

Figure S11. a) UV-Vis absorption spectral and b) emission spectral changes of **2** (chloroform, 0.05 mM) by gradual titration of **4** (1.00 mM). K_a for complex **2**/**4** is determined to be (6.02 ± 0.97) × 10^5 M^{-1}, by fitting the collected absorbance data at 460 nm with 1 : 1 model.

*10. ITC measurements for complexes **1/4** and **2/4***

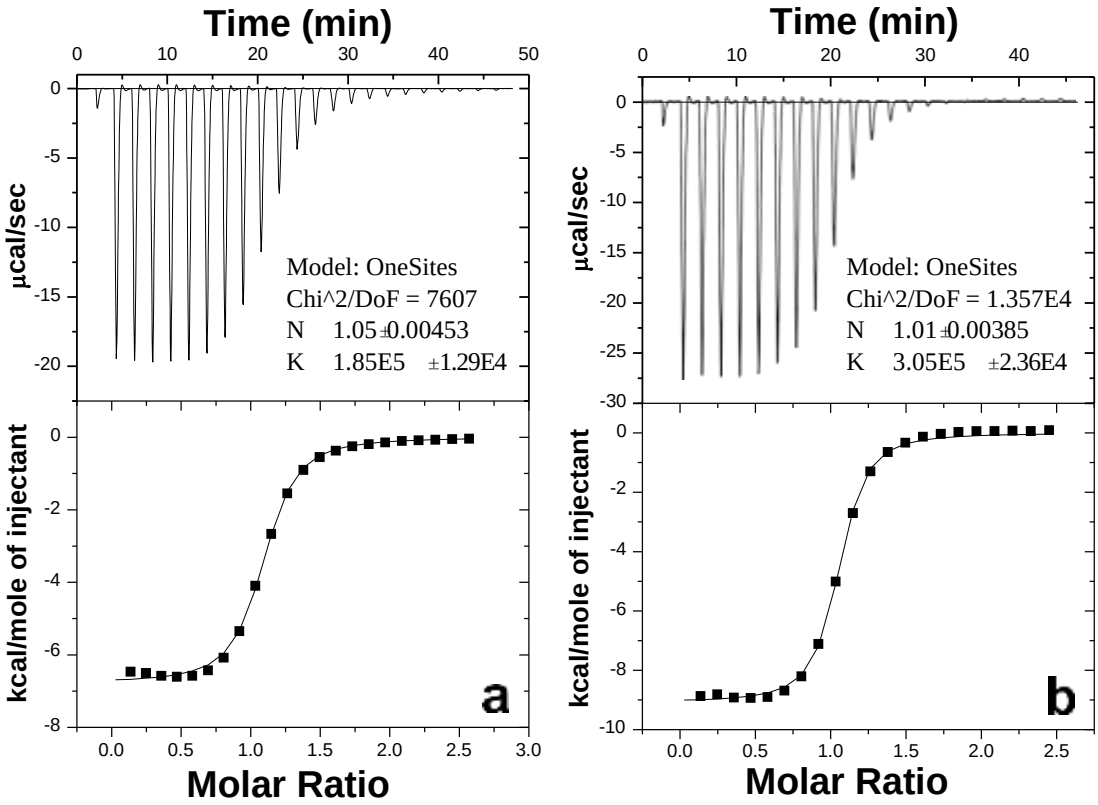

Figure S12. ITC data for titration of **4** (4.00 mM in chloroform) into the chloroform solution of a) **1** (0.20 mM) and b) **2** (0.20 mM).

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*11. Temperature-dependent UV-Vis titrations for complexes **1/3** and **2/3***

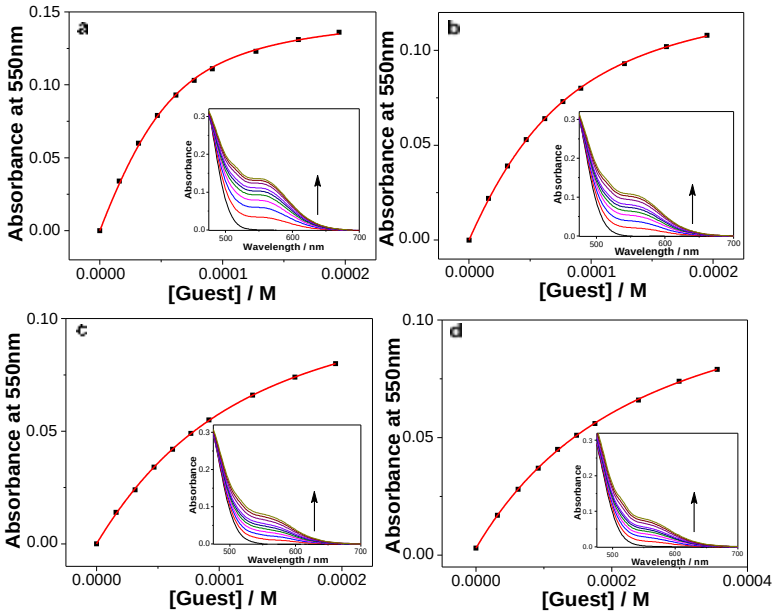


Figure S13. Non-linear fitting curves of UV-Vis absorbance at 550 nm at different temperatures: a) 30 °C, $K_a = (4.05 \pm 0.56) \times 10^5\ M^{-1}$ b) 45 °C, $K_a = (1.30 \pm 0.05) \times 10^5\ M^{-1}$ c) 60 °C, $K_a = (6.52 \pm 0.16) \times 10^4\ M^{-1}$ d) 75 °C. $K_a = (2.60 \pm 0.05) \times 10^4\ M^{-1}$ The inset figure indicates the absorption spectral changes of **1** (1,2-dichloroethane, 0.01 mM) by gradual titration of **3**.

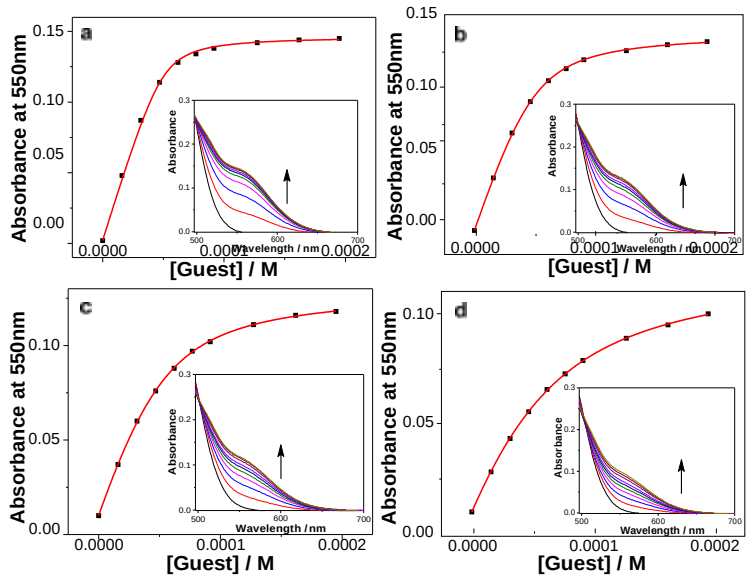


Figure S14. Non-linear fitting curves of UV-Vis absorbance at 550 nm at different temperatures: a) 30 °C, $K_a = (4.97 \pm 0.26) \times 10^4\ M^{-1}$ b) 45 °C, $K_a = (2.19 \pm 0.06) \times 10^4\ M^{-1}$ c) 60 °C, $K_a = (1.18 \pm 0.04) \times 10^4\ M^{-1}$ d) 75 °C, $K_a = (4.88 \pm 0.11) \times 10^3\ M^{-1}$ The inset figure indicates the absorption spectral changes of **2** (1,2-dichloroethane, 0.01 mM) by gradual titration of **3**.

12. Reversible complexation for the three-component recognition system

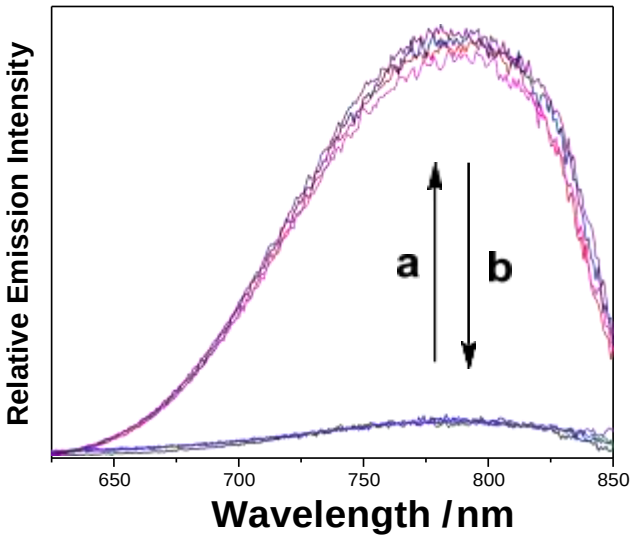


Figure S15. Fluorescent spectral changes upon successive (a) addition and (b) removal of 2% amount of HFIP in a 1 : 1 : 10 mixture **2**, **3** and **4** in chloroform.

13. *DFT calculations for complexes **1/3** and **1/4***

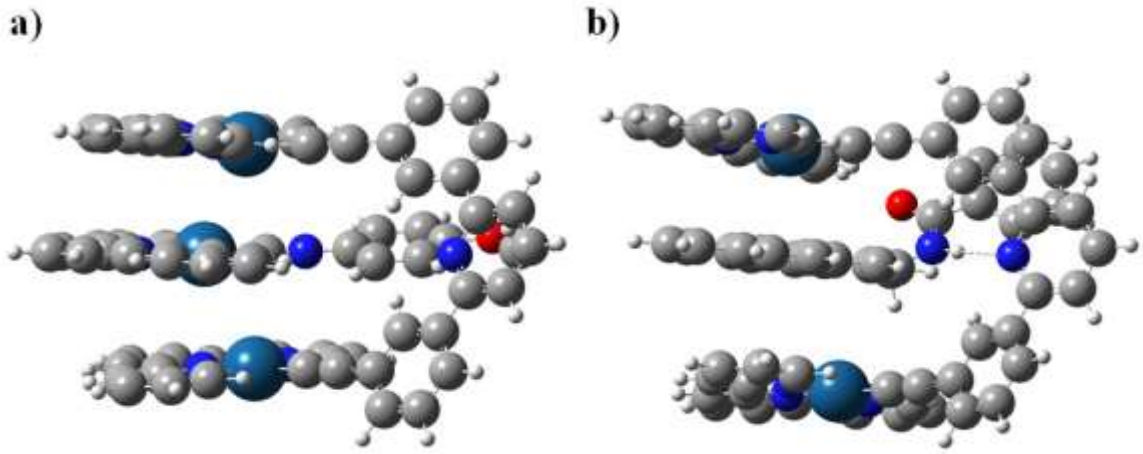
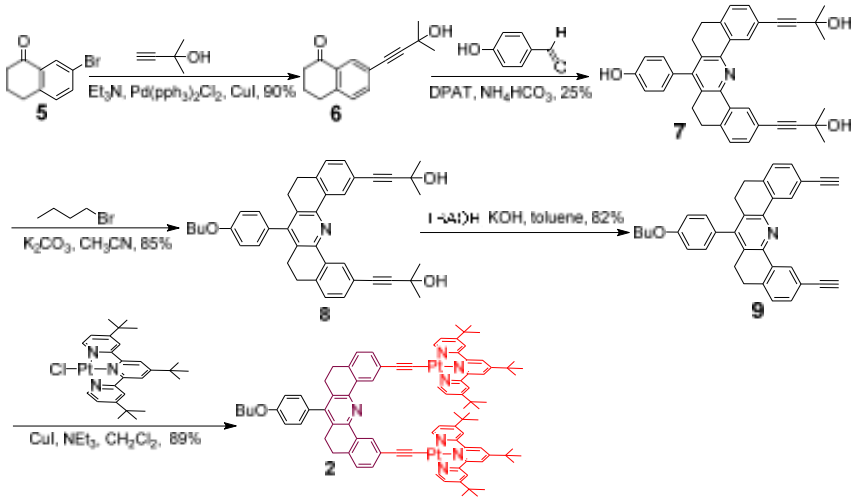


Figure S16. Optimized structures of a) complex **1/3** and b) **1/4** by DFT method.

*14. Synthetic route to molecular tweezer **2***



Scheme S1. Synthetic route to the targeted molecular tweezer **2**.

*14.1. Spectral data of compound **6***

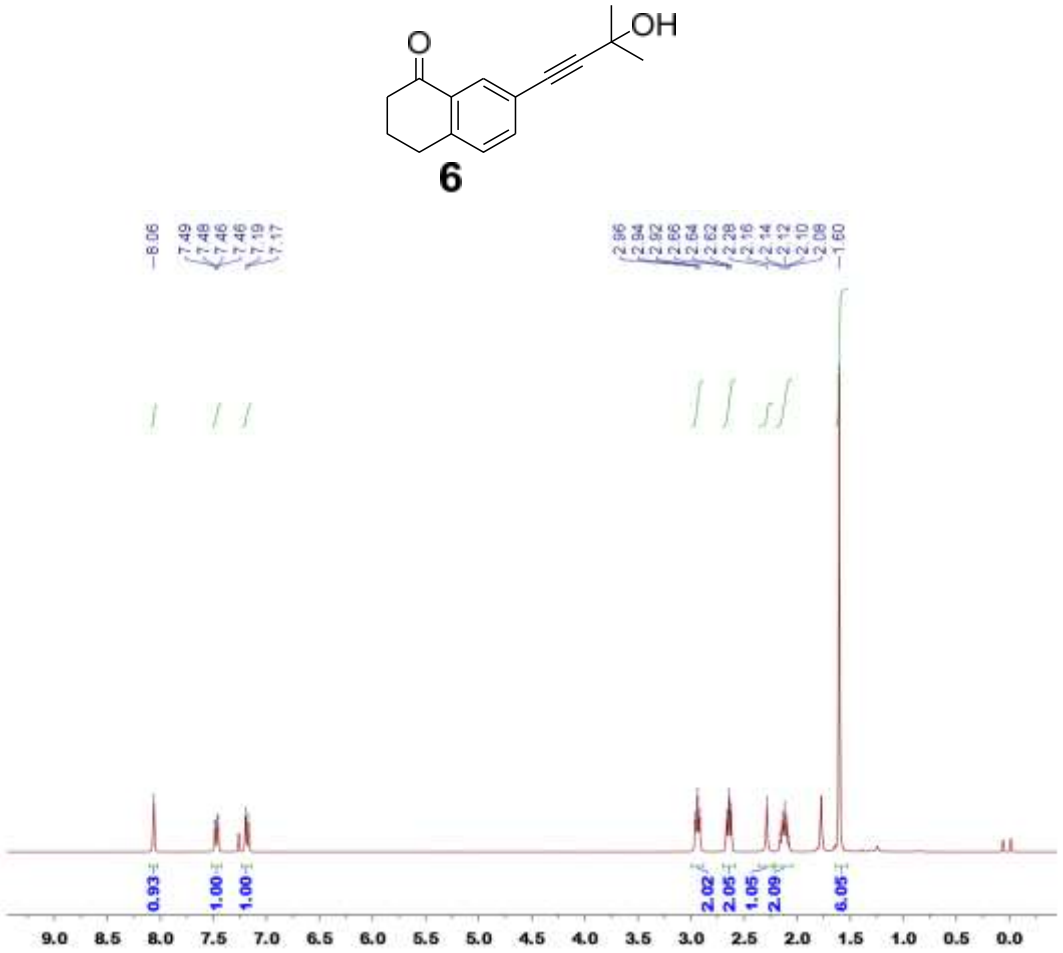


Figure S17. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, room temperature) of compound **6**.

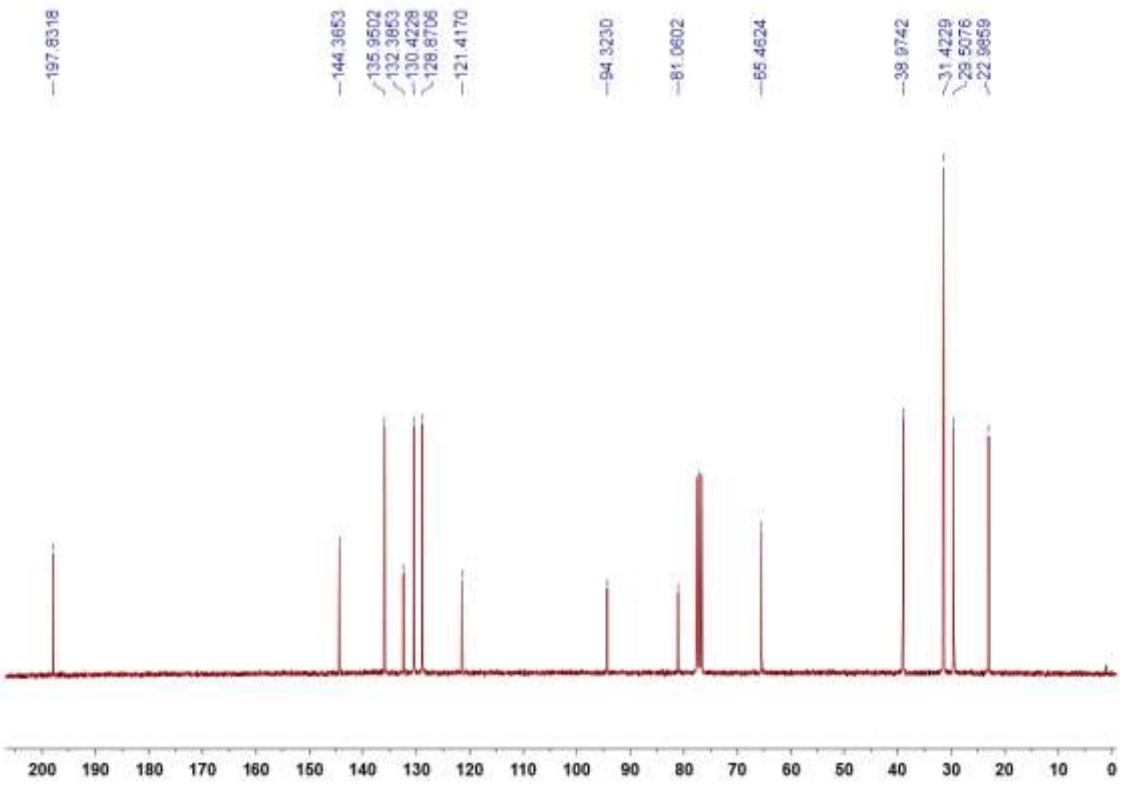


Figure S18. ^{13}C NMR spectrum (75 MHz, $CDCl_3$, room temperature) of compound **6**.

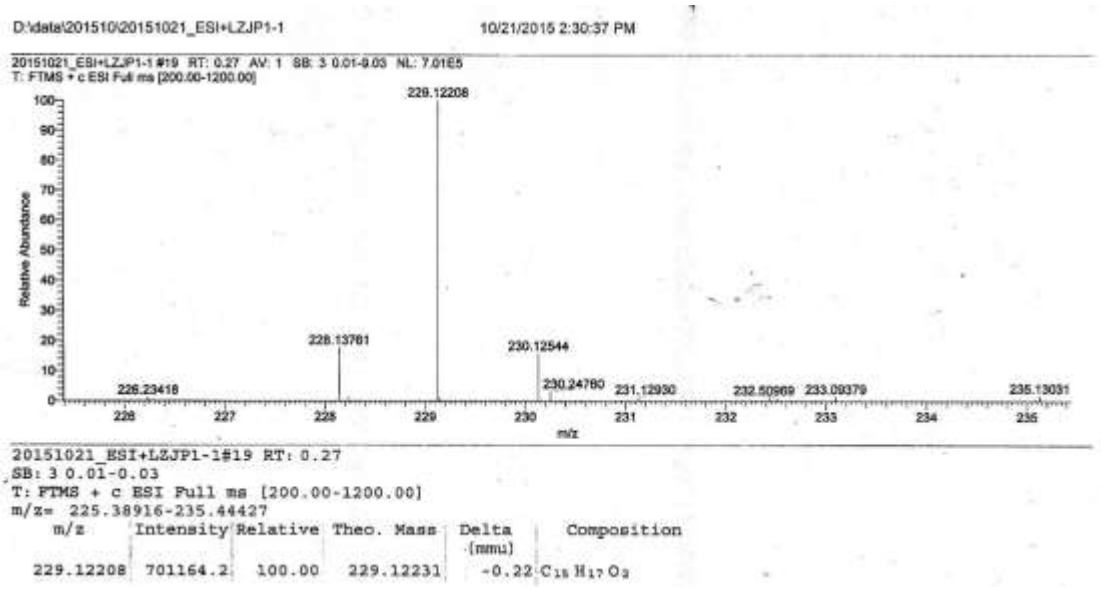
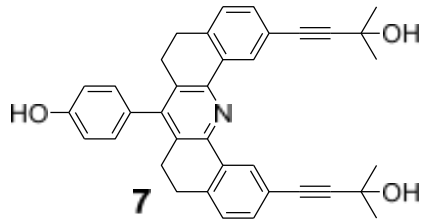


Figure S19. Electrospray ionization spectrum of compound **6**.

14.2. *Spectral data of compound **7***



7

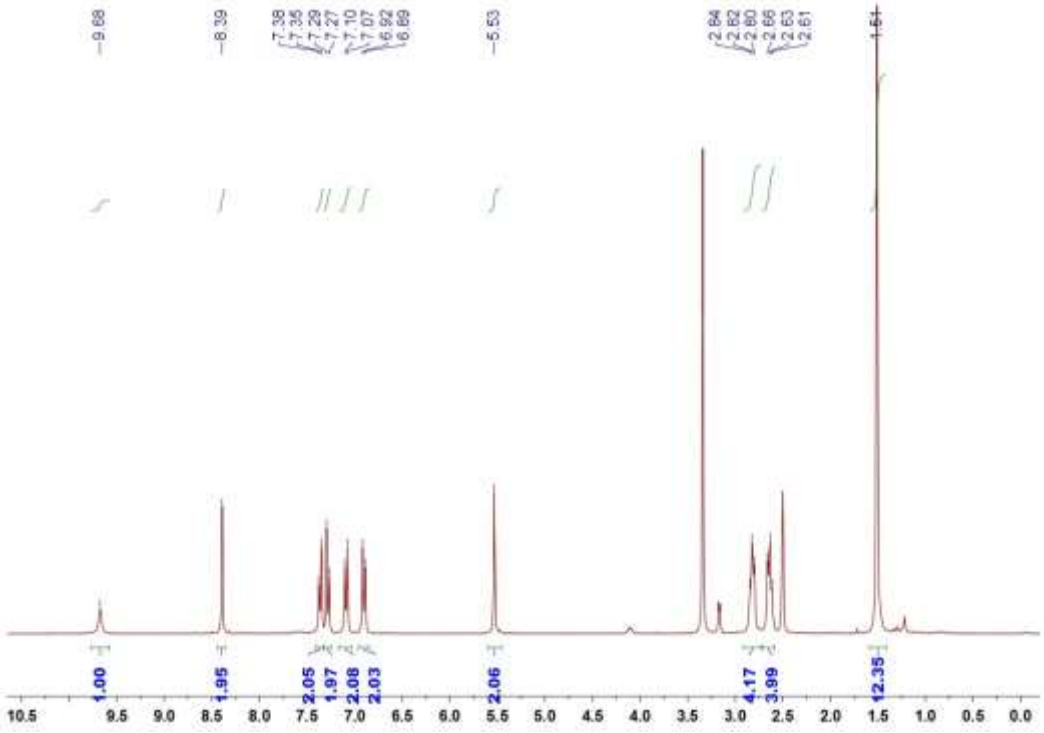


Figure S20. ^{1}H NMR spectrum (300 MHz, DMSO-d_6, room temperature) of compound **7**.

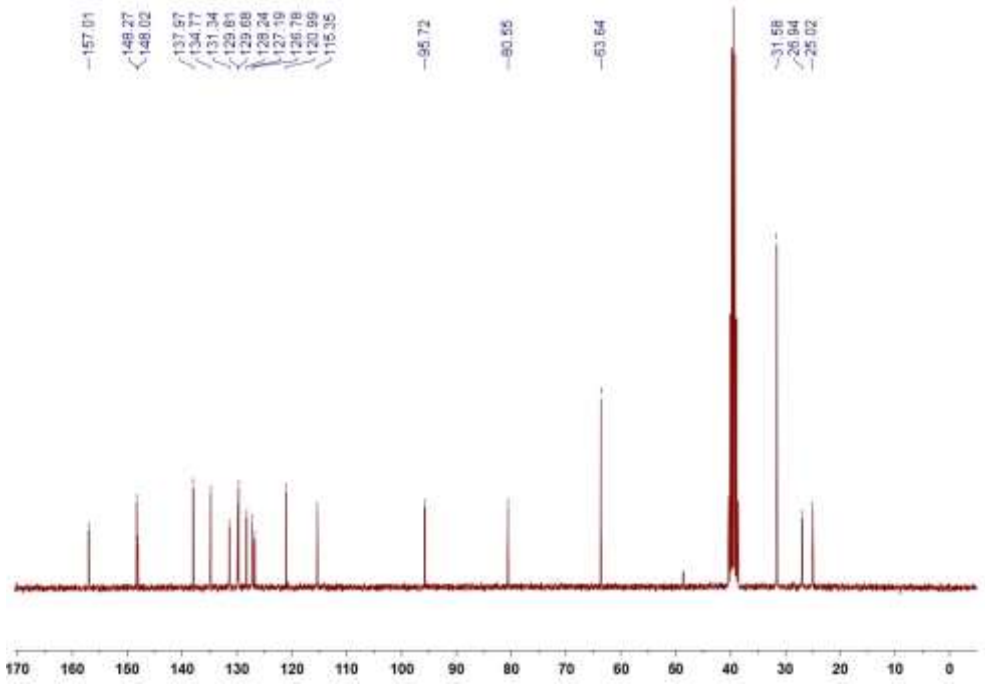


Figure S21. ^{13}C NMR spectrum (75 MHz, DMSO-d_6, room temperature) of compound **7**.

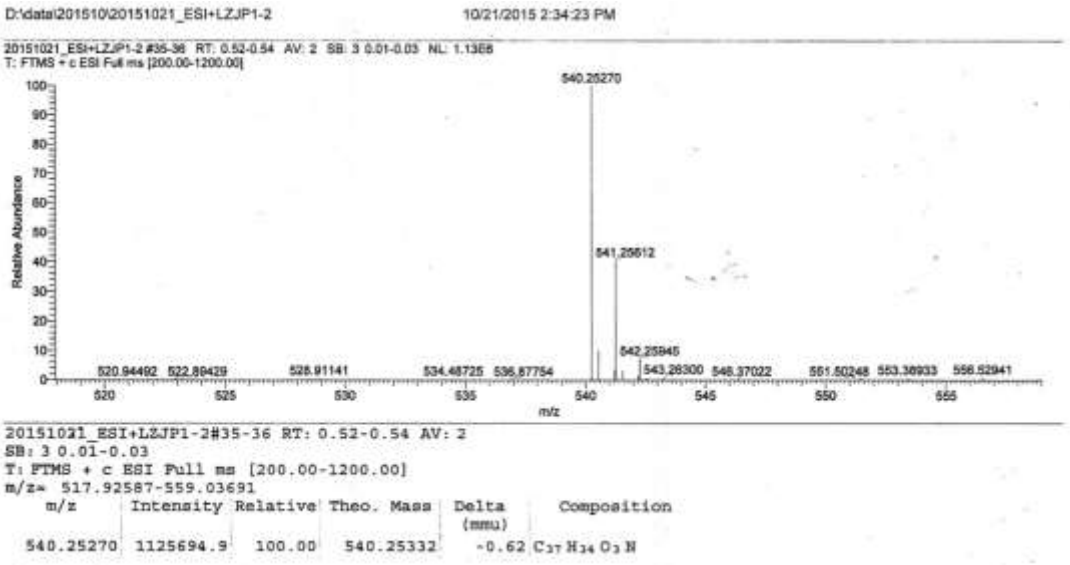
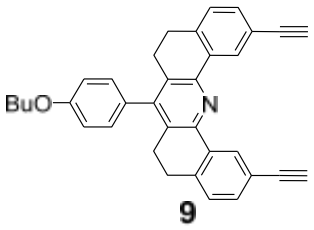


Figure S22. Electrospray ionization spectrum of compound **7**.

*14.3. Spectral data of compound **9***



9

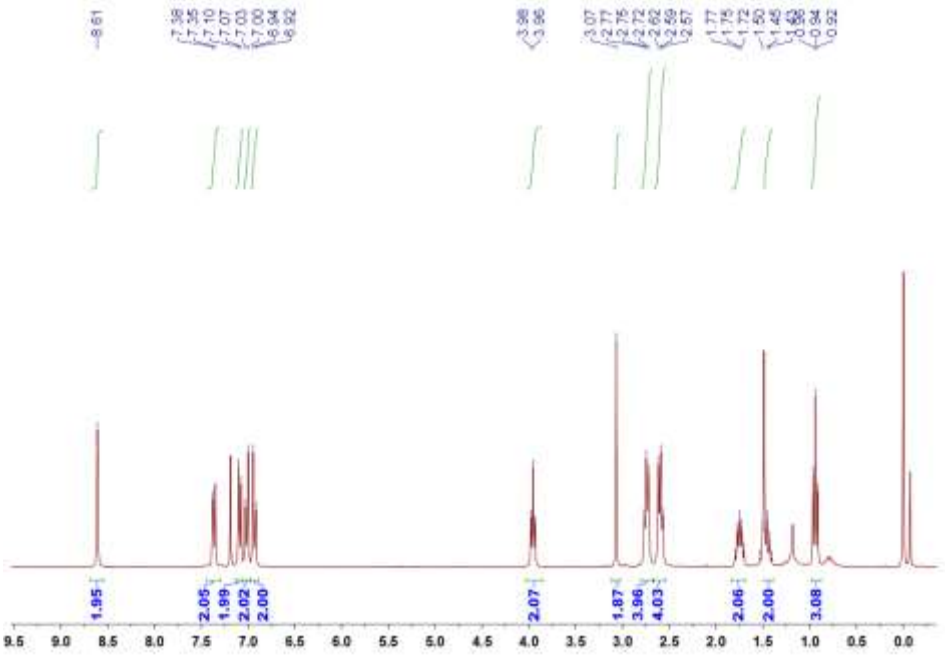


Figure S23. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, room temperature) of compound **9**.

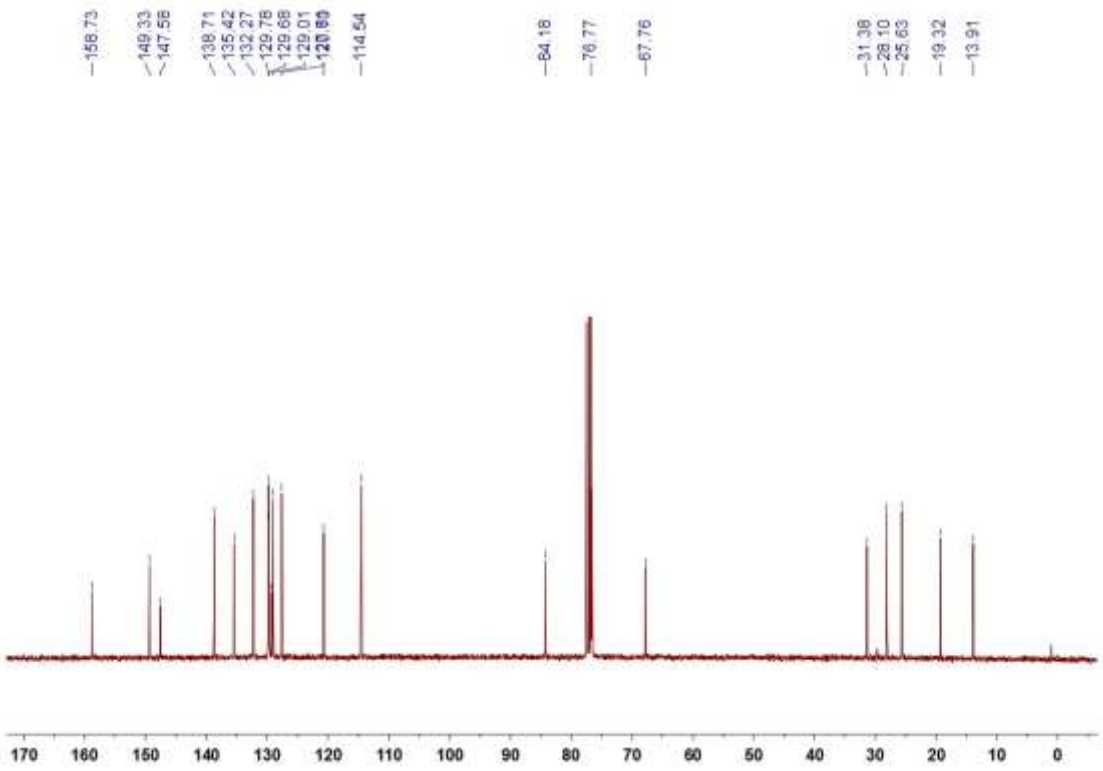


Figure S24. ^{13}C NMR spectrum (75 MHz, $CDCl_3$, room temperature) of compound **9**.

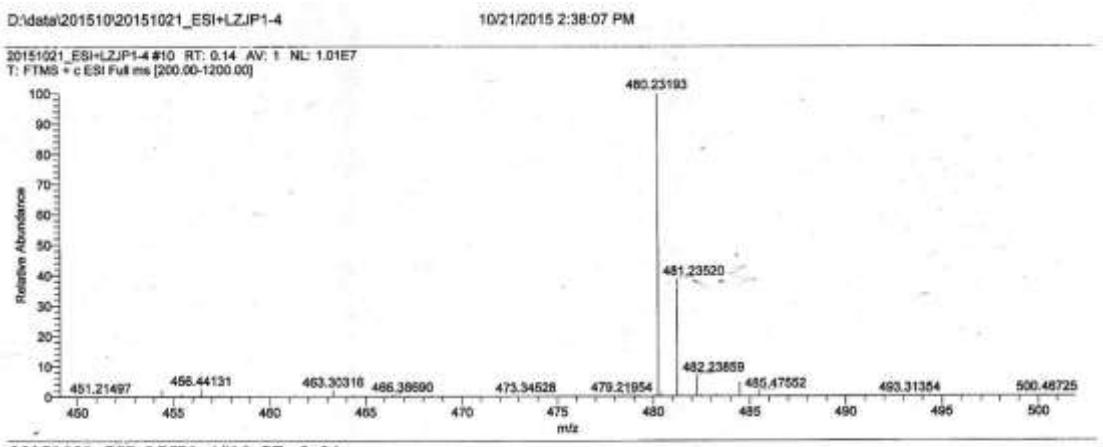


Figure S25. Electrospray ionization spectrum of compound **9**.

*14.4. Spectral data of compound **2***

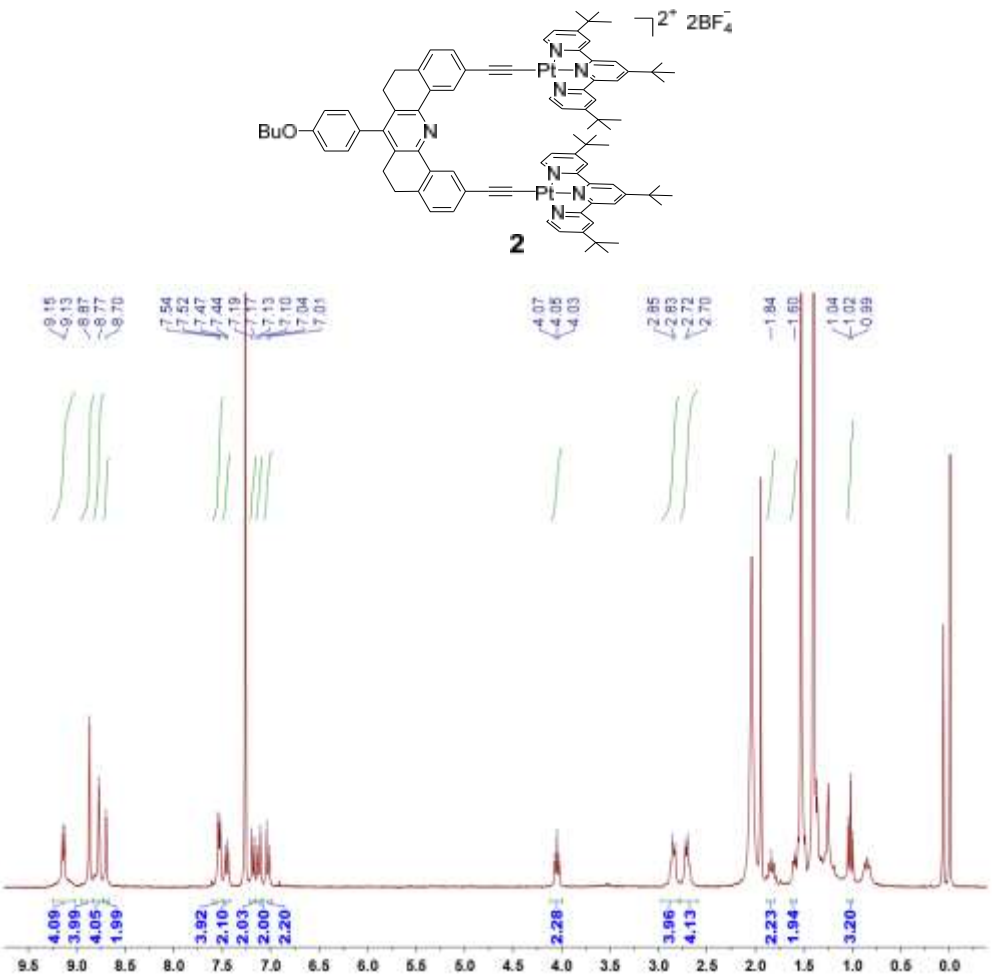


Figure S26. ^{1}H NMR spectrum (300 MHz, $CDCl_3$, room temperature) of compound **2**.

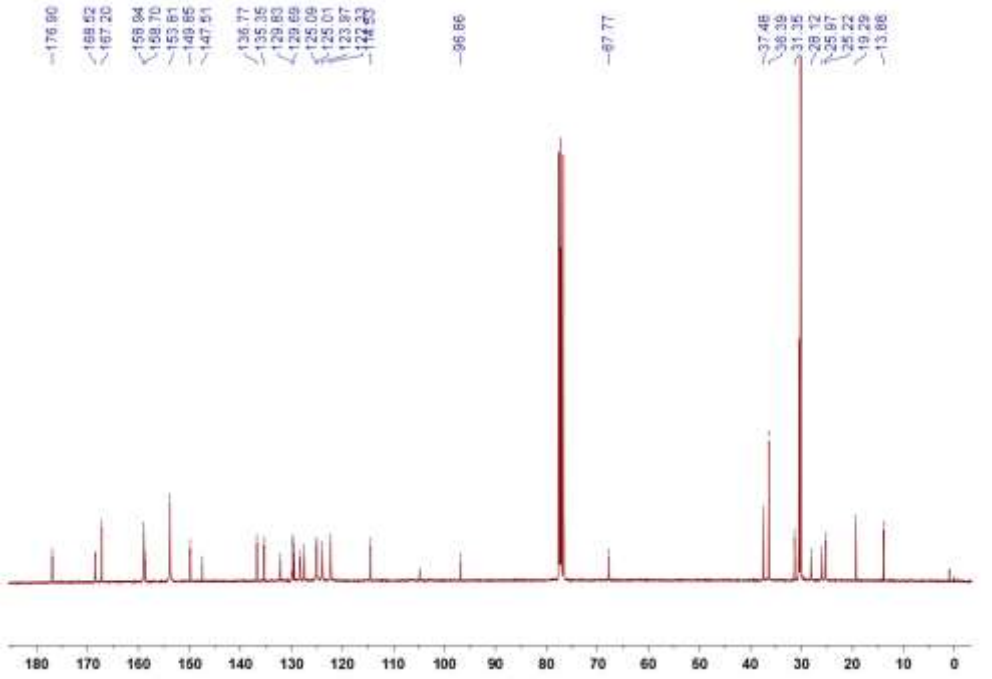


Figure S27. ^{13}C NMR spectrum (75 MHz, $CDCl_3$, room temperature) of compound **2**.

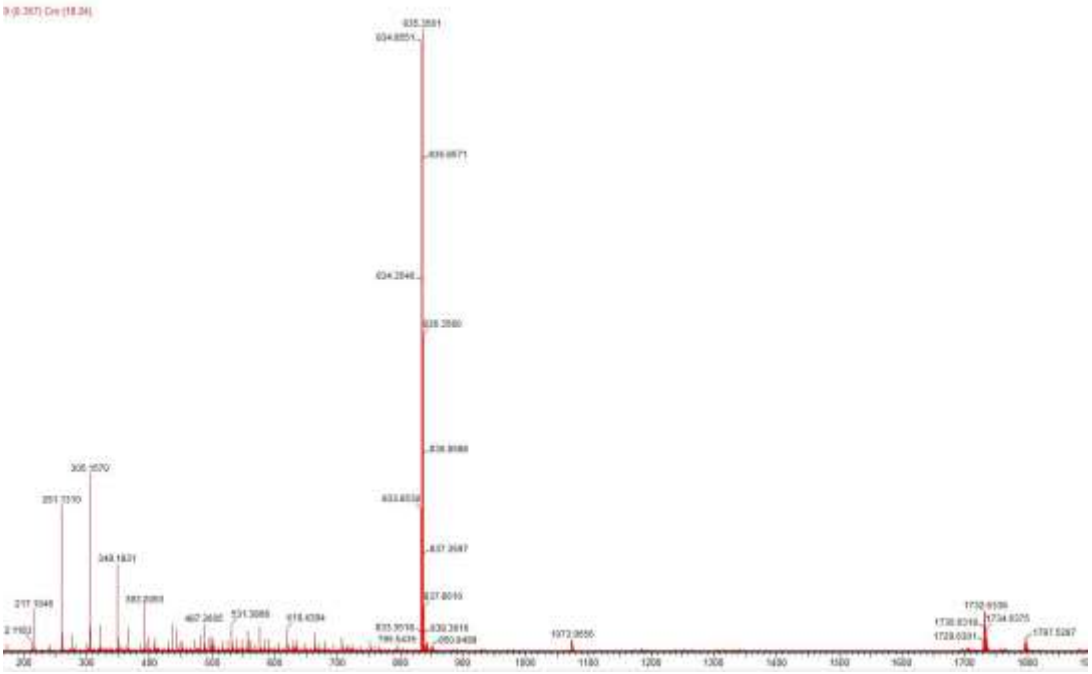


Figure S28. Electrospray ionization spectrum of compound **2**.

15. Atom coordination data for the DFT optimized complexes

Complex 2/4

SCF Done: E(PBE-PBE) = -3770.93069891 a.u.

Stoichiometry $C_{79}H_{54}N_8OPt_2(2+)$

Framework group $C1[X(C_{79}H_{54}N_8OPt_2)]$

Deg. of freedom 426

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	-1.309806	-3.566909	0.293099

2	78	0	-1.587993	3.765279	-0.478531
3	7	0	-1.950271	-4.439176	-1.430575
4	7	0	-3.228955	-3.797861	0.738162
5	7	0	-1.303174	-2.828904	2.186708
6	7	0	-2.116651	3.096197	-2.325393
7	7	0	-3.552255	3.655961	-0.232656
8	7	0	-1.727926	4.497419	1.416114
9	7	0	5.248121	0.396355	-0.913707
10	6	0	0.608466	-3.476460	-0.120294
11	6	0	1.811999	-3.455580	-0.426158
12	6	0	3.182900	-3.393133	-0.815055
13	6	0	3.832542	-4.511128	-1.396393
14	1	0	3.286697	-5.456303	-1.505862
15	6	0	5.163646	-4.408318	-1.811711
16	6	0	5.875119	-3.202026	-1.701568
17	6	0	5.231462	-2.070900	-1.130217
18	6	0	3.910513	-2.190788	-0.669752
19	1	0	3.436076	-1.349074	-0.168274
20	6	0	5.949297	-0.767695	-1.092279
21	6	0	7.359961	-0.769117	-1.261021
22	6	0	8.027010	0.461772	-1.331337
23	1	0	9.111420	0.485734	-1.478862
24	6	0	7.312423	1.663296	-1.224109
25	6	0	5.917144	1.587927	-0.988440
26	6	0	5.155674	2.853360	-0.826547
27	6	0	5.851438	4.054378	-0.514901
28	6	0	5.119068	5.242137	-0.334698
29	6	0	3.722928	5.256759	-0.432210
30	1	0	3.164363	6.183159	-0.281913
31	6	0	3.020080	4.065045	-0.743881

32	6	0	3.759129	2.878231	-0.966958
33	1	0	3.236941	1.966459	-1.261878
34	6	0	1.593370	4.032389	-0.771114
35	6	0	0.356556	3.938337	-0.713225
36	6	0	-1.185014	-4.742188	-2.518984
37	1	0	-0.128045	-4.484338	-2.429195
38	6	0	-1.735197	-5.352615	-3.649892
39	1	0	-1.090431	-5.592150	-4.496582
40	6	0	-3.106443	-5.659247	-3.670408
41	6	0	-3.896261	-5.349436	-2.553615
42	1	0	-4.961042	-5.588307	-2.545297
43	6	0	-3.316085	-4.740790	-1.433112
44	6	0	-4.036831	-4.398731	-0.192774
45	6	0	-5.376477	-4.649996	0.137838
46	1	0	-6.045169	-5.135972	-0.574451
47	6	0	-5.839286	-4.286704	1.416774
48	6	0	-4.976435	-3.691789	2.356703
49	1	0	-5.337842	-3.439340	3.354552
50	6	0	-3.641569	-3.451688	1.998939
51	6	0	-2.549929	-2.897092	2.820696
52	6	0	-2.680224	-2.478906	4.149089
53	1	0	-3.650437	-2.555696	4.643544
54	6	0	-1.564081	-1.974803	4.839131
55	6	0	-0.332172	-1.880125	4.177112
56	1	0	0.571515	-1.474035	4.631491
57	6	0	-0.230345	-2.322472	2.851640
58	1	0	0.714832	-2.261194	2.314425
59	6	0	-1.280904	2.894364	-3.384788
60	1	0	-0.222812	3.071596	-3.188673
61	6	0	-1.772208	2.502904	-4.634616

62	1	0	-1.075912	2.365302	-5.463122
63	6	0	-3.152069	2.308209	-4.803414
64	6	0	-4.013351	2.507956	-3.714064
65	1	0	-5.090078	2.371683	-3.825072
66	6	0	-3.493777	2.905972	-2.477545
67	6	0	-4.307353	3.210919	-1.285272
68	6	0	-5.700627	3.148767	-1.135527
69	1	0	-6.333727	2.796874	-1.951859
70	6	0	-6.271256	3.560356	0.083796
71	6	0	-5.465802	4.030806	1.139756
72	1	0	-5.919322	4.368281	2.072941
73	6	0	-4.074800	4.071966	0.963137
74	6	0	-3.039049	4.545815	1.901475
75	6	0	-3.292103	5.044055	3.184822
76	1	0	-4.318263	5.087310	3.553615
77	6	0	-2.230568	5.496368	3.982447
78	6	0	-0.920526	5.446763	3.478188
79	1	0	-0.073536	5.800097	4.067211
80	6	0	-0.698688	4.944353	2.192727
81	1	0	0.290738	4.887235	1.735342
82	6	0	7.362896	4.019233	-0.357921
83	1	0	7.781317	5.026585	-0.513631
84	1	0	7.616447	3.698981	0.671585
85	6	0	7.975577	3.021146	-1.367809
86	1	0	7.804682	3.400337	-2.397102
87	1	0	9.064797	2.930191	-1.213333
88	1	0	5.657262	6.169780	-0.103103
89	1	0	5.666678	-5.282853	-2.249739
90	6	0	7.303427	-3.084964	-2.209889
91	1	0	7.787707	-4.077420	-2.204759

92	1	0	7.293764	-2.713678	-3.255299
93	6	0	8.094838	-2.094733	-1.325754
94	1	0	9.116082	-1.948457	-1.717425
95	1	0	8.168741	-2.509055	-0.297167
96	1	0	-6.877129	-4.487267	1.690201
97	1	0	-1.664190	-1.660261	5.879613
98	1	0	-3.553670	-6.142111	-4.540965
99	1	0	-3.555826	2.015062	-5.773950
100	1	0	-7.355594	3.527950	0.207555
101	1	0	-2.425327	5.890697	4.980512
102	6	0	-1.537800	-0.095695	-0.487950
103	6	0	-0.665155	0.404841	0.548209
104	6	0	-0.994893	-0.500453	-1.755881
105	6	0	-2.951939	-0.194317	-0.265280
106	6	0	0.738671	0.476196	0.305282
107	6	0	-1.271810	0.797946	1.801217
108	6	0	0.398113	-0.399777	-1.959916
109	6	0	-1.883181	-1.007087	-2.773205
110	6	0	-3.518081	0.217211	0.992169
111	6	0	-3.817134	-0.709250	-1.297153
112	6	0	1.237863	0.076600	-0.948563
113	6	0	1.699039	1.066114	1.344563
114	6	0	-2.627161	0.709282	2.013307
115	1	0	-0.632816	1.165470	2.606142
116	1	0	0.824924	-0.720213	-2.915224
117	6	0	-3.235253	-1.113599	-2.554623
118	1	0	-1.448374	-1.310902	-3.731109
119	6	0	-4.915022	0.111190	1.192051
120	6	0	-5.207900	-0.800695	-1.049595
121	1	0	2.314103	0.120242	-1.133364

122	1	0	1.850902	2.135130	1.107714
123	1	0	1.266436	0.961354	2.351227
124	7	0	3.017215	0.411710	1.434621
125	1	0	-3.054619	1.001021	2.978563
126	1	0	-3.899680	-1.502148	-3.333809
127	6	0	-5.746862	-0.394500	0.180973
128	1	0	-5.340365	0.425320	2.150528
129	1	0	-5.861739	-1.195490	-1.833968
130	6	0	3.220730	-0.521700	2.430119
131	1	0	3.757389	0.621205	0.741406
132	1	0	-6.823482	-0.474536	0.353817
133	8	0	2.259256	-0.946912	3.141854
134	6	0	4.624177	-0.988249	2.647071
135	6	0	5.758137	-0.240059	2.271175
136	6	0	4.788075	-2.204003	3.341609
137	6	0	7.043226	-0.730136	2.550585
138	1	0	5.645182	0.735183	1.793252
139	6	0	6.070036	-2.695116	3.612336
140	1	0	3.891134	-2.741366	3.656894
141	6	0	7.201701	-1.960485	3.211310
142	1	0	7.920102	-0.144010	2.264897
143	1	0	6.193241	-3.643263	4.140808
144	1	0	8.203875	-2.336802	3.432090

Complex 2/3

SCF Done: E(PBE-PBE) = -3983.19012221 a.u.

Stoichiometry $C_{80}H_{55}N_9OPt_3(2+)$

Framework group C1[X($C_{80}H_{55}N_9OPt_3$)]

Deg. of freedom 438

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	1.235985	3.238446	0.617760
2	78	0	0.959351	-3.344904	-0.571322
3	7	0	1.989914	3.804584	-1.186132
4	7	0	3.165120	3.317169	1.079911
5	7	0	1.124428	2.853750	2.617394
6	7	0	1.129383	-2.959437	-2.565076
7	7	0	2.925389	-3.521992	-0.772301
8	7	0	1.435321	-3.926585	1.318271
9	7	0	-5.640355	0.248540	-0.946879
10	6	0	-0.675102	3.386336	0.165105
11	6	0	-1.845528	3.549095	-0.217963
12	6	0	-3.185357	3.674793	-0.700867
13	6	0	-3.689817	4.913485	-1.184286
14	1	0	-3.046281	5.796299	-1.164112
15	6	0	-5.001495	5.001106	-1.669651
16	6	0	-5.849953	3.877286	-1.686017
17	6	0	-5.353112	2.643882	-1.194223
18	6	0	-4.037679	2.546987	-0.715626
19	6	0	-6.226730	1.450028	-1.170136
20	6	0	-7.629030	1.597668	-1.314861
21	6	0	-8.419191	0.436432	-1.248164
22	1	0	-9.505142	0.510064	-1.367265

23	6	0	-7.824181	-0.816644	-1.021069
24	6	0	-6.417678	-0.857465	-0.857305
25	6	0	-5.743636	-2.144864	-0.579540
26	6	0	-6.499923	-3.257628	-0.131235
27	6	0	-5.824344	-4.453130	0.183282
28	6	0	-4.429267	-4.547693	0.080464
29	1	0	-3.916345	-5.480650	0.326150
30	6	0	-3.668852	-3.428354	-0.354815
31	6	0	-4.349351	-2.236194	-0.692975
32	1	0	-3.797164	-1.350669	-1.012964
33	6	0	-2.241814	-3.448711	-0.407726
34	6	0	-1.001614	-3.386810	-0.432050
35	6	0	1.275501	4.037956	-2.324561
36	1	0	0.200580	3.867237	-2.248964
37	6	0	1.900932	4.472640	-3.498174
38	1	0	1.294766	4.661274	-4.385102
39	6	0	3.292395	4.663062	-3.511321
40	6	0	4.032616	4.402597	-2.347957
41	1	0	5.114827	4.543901	-2.335820
42	6	0	3.378862	3.974062	-1.185959
43	6	0	4.044559	3.704151	0.101466
44	6	0	5.402554	3.832514	0.428675
45	1	0	6.127957	4.147741	-0.322509
46	6	0	5.812395	3.568232	1.749818
47	6	0	4.878468	3.198446	2.736430
48	1	0	5.200852	3.020884	3.763190
49	6	0	3.526396	3.085083	2.381640
50	6	0	2.369427	2.808094	3.250641
51	6	0	2.448138	2.567017	4.627967
52	1	0	3.424795	2.535576	5.113387

53	6	0	1.275988	2.371658	5.372956
54	6	0	0.031375	2.421713	4.722178
55	1	0	-0.902246	2.283025	5.269674
56	6	0	-0.013302	2.668889	3.346513
57	1	0	-0.945546	2.744378	2.787249
58	6	0	0.108448	-2.682068	-3.426241
59	1	0	-0.886663	-2.646264	-2.981310
60	6	0	0.343233	-2.479569	-4.790343
61	1	0	-0.498011	-2.261671	-5.449140
62	6	0	1.654907	-2.562808	-5.285710
63	6	0	2.707930	-2.837156	-4.400638
64	1	0	3.734359	-2.911164	-4.764237
65	6	0	2.441865	-3.033340	-3.039389
66	6	0	3.460181	-3.364017	-2.025218
67	6	0	4.835156	-3.577177	-2.200774
68	1	0	5.292137	-3.472165	-3.185557
69	6	0	5.613094	-3.953209	-1.088153
70	6	0	5.026391	-4.129882	0.179755
71	1	0	5.630958	-4.450913	1.029231
72	6	0	3.647854	-3.914548	0.324435
73	6	0	2.805888	-4.119749	1.516914
74	6	0	3.281658	-4.530982	2.767845
75	1	0	4.352754	-4.676226	2.914786
76	6	0	2.381209	-4.762217	3.817803
77	6	0	1.006889	-4.570032	3.600018
78	1	0	0.278316	-4.753417	4.390987
79	6	0	0.563298	-4.147623	2.343247
80	1	0	-0.488595	-3.988186	2.101337
81	6	0	-7.999221	-3.084994	0.074728
82	1	0	-8.508344	-4.063746	0.036171

83	1	0	-8.165283	-2.654411	1.085291
84	6	0	-8.602948	-2.121743	-0.980371
85	1	0	-8.545028	-2.603926	-1.977145
86	1	0	-9.666771	-1.927490	-0.758029
87	1	0	-6.401026	-5.320342	0.518474
88	1	0	-5.376444	5.958936	-2.042111
89	6	0	-7.256789	3.915210	-2.266305
90	1	0	-7.641311	4.949932	-2.271018
91	1	0	-7.216064	3.562488	-3.317068
92	6	0	-8.213173	2.993496	-1.464950
93	1	0	-9.198880	2.943766	-1.960104
94	1	0	-8.362269	3.424460	-0.453855
95	1	0	6.865534	3.671886	2.017816
96	1	0	1.333216	2.191774	6.448146
97	1	0	3.796491	5.013855	-4.413943
98	1	0	1.855190	-2.421194	-6.349585
99	1	0	6.682234	-4.133634	-1.215937
100	1	0	2.747630	-5.095578	4.790466
101	78	0	1.183321	-0.009896	0.017493
102	6	0	2.404209	-0.467525	1.641095
103	6	0	0.578701	0.471279	-1.912358
104	7	0	2.987039	0.043126	-0.892620
105	6	0	-0.523990	-0.045892	0.885123
106	6	0	3.802790	-0.489910	1.282066
107	6	0	2.083317	-0.742244	2.989839
108	6	0	1.694516	0.575138	-2.822336
109	6	0	-0.708992	0.729388	-2.432422
110	6	0	3.024046	0.336809	-2.238775
111	6	0	4.108132	-0.199606	-0.130462
112	7	0	-1.575505	-0.071426	1.442021

113	6	0	4.801664	-0.771609	2.240044
114	6	0	3.082676	-1.020921	3.941968
115	1	0	1.032717	-0.735031	3.300712
116	6	0	1.500345	0.911309	-4.181191
117	6	0	-0.896266	1.067844	-3.786352
118	1	0	-1.577766	0.686004	-1.768508
119	6	0	4.280558	0.387705	-2.876743
120	6	0	5.369496	-0.144072	-0.753916
121	6	0	-2.802211	-0.100692	2.086256
122	6	0	4.442111	-1.034846	3.570082
123	1	0	5.859253	-0.782119	1.955298
124	1	0	2.804823	-1.230255	4.979929
125	6	0	0.205695	1.156963	-4.661911
126	1	0	2.352929	0.988612	-4.864753
127	1	0	-1.905206	1.271629	-4.158819
128	6	0	5.444103	0.149426	-2.126868
129	1	0	4.339907	0.620905	-3.940948
130	1	0	6.274312	-0.326937	-0.172702
131	6	0	-3.470168	1.109190	2.400143
132	6	0	-3.411802	-1.332239	2.398832
133	1	0	5.213999	-1.248953	4.314115
134	1	0	0.052059	1.420784	-5.711672
135	1	0	6.420631	0.195352	-2.616462
136	6	0	-4.716087	1.075004	3.014615
137	1	0	-3.022078	2.062335	2.111162
138	6	0	-4.668640	-1.361789	3.008841
139	1	0	-2.915037	-2.260895	2.114693
140	6	0	-5.336685	-0.160028	3.322526
141	1	0	-5.258027	1.992688	3.246370
142	1	0	-5.132421	-2.328384	3.207235

143	8	0	-6.581396	-0.071074	3.907398
144	6	0	-7.311544	-1.331402	4.148542
145	1	0	-7.504573	-1.864321	3.199046
146	1	0	-6.761266	-1.991162	4.843443
147	1	0	-8.260076	-1.016936	4.603655
148	1	0	-3.695538	1.577440	-0.349956

Complex 1/4

SCF Done: E(PBE-PBE) = -3617.08773504 a.u.

Stoichiometry $C_{75}H_{50}N_8OPt_2(2+)$

Framework group C1[X($C_{75}H_{50}N_8OPt_2$)]

Deg. of freedom 402

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	78	0	3.815530	0.596975	0.854991
2	78	0	-3.523784	-2.747168	-0.382990
3	7	0	5.026526	0.792864	-0.764975
4	7	0	5.009501	-0.957613	1.158012
5	7	0	2.996118	-0.118303	2.571163
6	7	0	-1.963586	-3.426707	-1.504718
7	7	0	-3.122850	-4.421847	0.605485
8	7	0	-4.936715	-2.619036	1.080079
9	7	0	-2.355384	4.711259	-1.355612

10	6	0	2.758382	2.243410	0.713844
11	6	0	2.142333	3.319396	0.742315
12	6	0	1.322395	4.483502	0.840185
13	6	0	1.505015	5.427497	1.883809
14	1	0	2.329392	5.291760	2.588835
15	6	0	0.624153	6.510636	2.008753
16	6	0	-0.451824	6.663576	1.120783
17	1	0	-1.170268	7.472611	1.271969
18	6	0	-0.645464	5.733428	0.073596
19	6	0	0.253042	4.662935	-0.070402
20	1	0	0.130509	3.952342	-0.886590
21	6	0	-1.795000	5.862674	-0.860285
22	6	0	-2.258630	7.139187	-1.241117
23	1	0	-1.756830	8.030634	-0.861759
24	6	0	-3.339085	7.242604	-2.125110
25	1	0	-3.725632	8.221639	-2.416435
26	6	0	-3.907238	6.071750	-2.643367
27	1	0	-4.759167	6.117982	-3.323476
28	6	0	-3.377050	4.821736	-2.264456
29	6	0	-3.907423	3.568944	-2.872035
30	6	0	-4.374883	3.564549	-4.206730
31	1	0	-4.356214	4.486657	-4.791895
32	6	0	-4.816560	2.372338	-4.799336
33	6	0	-4.774512	1.165843	-4.089947
34	1	0	-5.095732	0.231663	-4.554390
35	6	0	-4.303840	1.149456	-2.752433
36	6	0	-3.895435	2.363598	-2.149431
37	1	0	-3.564061	2.358028	-1.111354
38	6	0	-4.168823	-0.075536	-2.032895
39	6	0	-3.955937	-1.110277	-1.382379

40	6	0	4.938831	1.753940	-1.728147
41	1	0	4.146885	2.491238	-1.584383
42	6	0	5.823817	1.778236	-2.812716
43	1	0	5.727037	2.564196	-3.563439
44	6	0	6.822234	0.795652	-2.911638
45	6	0	6.913312	-0.195984	-1.921949
46	1	0	7.680436	-0.970437	-1.981084
47	6	0	6.014479	-0.194729	-0.848225
48	6	0	6.025281	-1.167491	0.262761
49	6	0	6.939827	-2.201898	0.513978
50	1	0	7.766387	-2.393947	-0.172757
51	6	0	6.785587	-2.976838	1.680547
52	6	0	5.737158	-2.723022	2.588795
53	1	0	5.640904	-3.313923	3.501796
54	6	0	4.835635	-1.683933	2.309588
55	6	0	3.675201	-1.222572	3.101546
56	6	0	3.221726	-1.815121	4.287663
57	1	0	3.767162	-2.662328	4.709016
58	6	0	2.068106	-1.320027	4.925063
59	6	0	1.376580	-0.241957	4.351746
60	1	0	0.455608	0.168347	4.771417
61	6	0	1.870264	0.349193	3.179794
62	1	0	1.340954	1.179393	2.707604
63	6	0	-1.388425	-2.794746	-2.568011
64	1	0	-1.835236	-1.839142	-2.846534
65	6	0	-0.288557	-3.347121	-3.235826
66	1	0	0.157917	-2.803381	-4.069498
67	6	0	0.230211	-4.579281	-2.808647
68	6	0	-0.362251	-5.234153	-1.716622
69	1	0	0.027201	-6.192270	-1.367668

70	6	0	-1.452948	-4.651914	-1.061773
71	6	0	-2.124397	-5.226370	0.122502
72	6	0	-1.862425	-6.438192	0.779773
73	1	0	-1.084066	-7.111629	0.417557
74	6	0	-2.630887	-6.778223	1.910481
75	6	0	-3.649525	-5.925790	2.379777
76	1	0	-4.244459	-6.202997	3.251550
77	6	0	-3.892769	-4.724228	1.697768
78	6	0	-4.912172	-3.692601	1.977522
79	6	0	-5.818522	-3.736848	3.043341
80	1	0	-5.792880	-4.577125	3.739463
81	6	0	-6.754831	-2.703756	3.209712
82	6	0	-6.771714	-1.637049	2.296777
83	1	0	-7.488243	-0.820112	2.394343
84	6	0	-5.853187	-1.620684	1.239958
85	1	0	-5.813991	-0.824994	0.493839
86	1	0	-1.175906	2.443207	-1.837668
87	6	0	-0.413023	1.659111	-1.874561
88	6	0	-0.309335	0.730985	-0.818209
89	6	0	0.437453	1.606515	-2.983466
90	6	0	0.659543	-0.313376	-0.899442
91	6	0	1.428663	0.606172	-3.090906
92	1	0	0.327906	2.338777	-3.788694
93	6	0	1.543664	-0.368718	-2.039967
94	6	0	0.799711	-1.344792	0.105929
95	6	0	2.304159	0.518746	-4.233768
96	6	0	2.531594	-1.403833	-2.147784
97	6	0	1.747341	-2.336260	0.002664
98	1	0	0.142452	-1.326766	0.979131
99	6	0	3.249219	-0.472060	-4.335497

100	1	0	2.188976	1.261138	-5.029047
101	6	0	2.651042	-2.402366	-1.118811
102	6	0	3.397452	-1.464676	-3.299124
103	1	0	1.836698	-3.095977	0.787861
104	1	0	3.900754	-0.534722	-5.212415
105	6	0	3.631049	-3.415031	-1.245821
106	6	0	4.356592	-2.501754	-3.386836
107	6	0	4.472332	-3.460500	-2.369496
108	1	0	3.720001	-4.171310	-0.458776
109	1	0	5.002939	-2.552634	-4.268301
110	1	0	5.214663	-4.258065	-2.459674
111	6	0	-1.308152	0.788347	0.334382
112	1	0	-2.241831	0.287946	0.009576
113	1	0	-0.918648	0.267609	1.222170
114	7	0	-1.625204	2.136779	0.848150
115	6	0	-1.369494	2.406332	2.175645
116	8	0	-0.723428	1.594016	2.912041
117	6	0	-1.933686	3.673492	2.736116
118	6	0	-2.960759	4.413388	2.117471
119	6	0	-1.452649	4.073759	3.998787
120	6	0	-3.481949	5.552399	2.748718
121	1	0	-3.367122	4.107799	1.151005
122	6	0	-1.967585	5.214209	4.624448
123	1	0	-0.676810	3.464314	4.466239
124	6	0	-2.985458	5.957073	3.999510
125	1	0	-4.283290	6.119258	2.268576
126	1	0	-1.586744	5.522587	5.600837
127	1	0	-3.398147	6.841445	4.490565
128	1	0	-1.918699	2.890525	0.208419
129	1	0	-5.172207	2.381710	-5.831670

130	1	0	0.759379	7.226148	2.823176
131	1	0	7.525440	0.801434	-3.747526
132	1	0	7.498892	-3.776180	1.893121
133	1	0	1.717540	-1.781171	5.851929
134	1	0	-7.462723	-2.734454	4.040588
135	1	0	-2.440025	-7.721103	2.426616
136	1	0	1.093436	-5.019992	-3.310936

Complex 1/3

SCF Done: E(PBE-PBE) = -3829.36146294 a.u.

Stoichiometry $C_{76}H_{51}N_9OPt_3(2+)$

Framework group C1[X($C_{76}H_{51}N_9OPt_3$)]

Deg. of freedom 414

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.454313	-1.427905	-1.291572
2	6	0	9.150257	-0.301418	-1.750216
3	6	0	8.498475	0.936976	-1.813676
4	6	0	7.151866	1.026537	-1.404371
5	7	0	6.486279	-0.066067	-0.930899
6	6	0	7.114354	-1.275046	-0.882937
7	6	0	6.376088	2.301006	-1.472490
8	6	0	5.039874	2.300571	-1.030275

9	6	0	4.248226	3.470682	-1.069082
10	6	0	4.818830	4.668841	-1.577475
11	6	0	6.145736	4.671577	-2.023909
12	6	0	6.923721	3.503521	-1.974175
13	6	0	2.899521	3.442689	-0.594870
14	6	0	1.724057	3.411368	-0.195928
15	78	0	-0.150325	3.384614	0.406082
16	7	0	0.118741	3.035467	2.392473
17	6	0	-1.079807	2.933837	3.107859
18	6	0	-1.053344	2.699655	4.487520
19	6	0	0.176362	2.575582	5.154058
20	6	0	1.369294	2.684477	4.422432
21	6	0	1.311516	2.915864	3.043238
22	6	0	-2.307908	3.113545	2.311620
23	7	0	-2.047263	3.388827	0.997877
24	6	0	-3.014655	3.594999	0.052961
25	6	0	-4.360470	3.519224	0.440100
26	6	0	-4.664267	3.233270	1.784780
27	6	0	-3.642952	3.030396	2.731379
28	6	0	-2.452586	3.862439	-1.284011
29	7	0	-1.057879	3.806182	-1.368614
30	6	0	-0.438464	4.049609	-2.557884
31	6	0	-1.169551	4.375682	-3.706365
32	6	0	-2.569750	4.444437	-3.637157
33	6	0	-3.211605	4.177768	-2.417424
34	6	0	-5.258780	-3.361991	-0.816359
35	6	0	-4.495138	-3.233166	-1.992642
36	6	0	-3.096648	-3.195454	-1.890249
37	7	0	-2.527275	-3.289646	-0.648619
38	6	0	-3.239019	-3.438641	0.511292

39	6	0	-4.639083	-3.466638	0.444286
40	6	0	-2.094886	-3.083832	-2.965903
41	7	0	-0.763286	-3.043482	-2.541253
42	6	0	0.239690	-2.966937	-3.461691
43	6	0	-0.031272	-2.937990	-4.834437
44	6	0	-1.362379	-2.988464	-5.277041
45	6	0	-2.397529	-3.056099	-4.332498
46	6	0	-2.370996	-3.579945	1.695259
47	7	0	-0.997640	-3.516246	1.440801
48	6	0	-0.107173	-3.697786	2.459951
49	6	0	-0.539762	-3.947316	3.767041
50	6	0	-1.916782	-3.997977	4.041995
51	6	0	-2.833645	-3.807425	2.996762
52	78	0	-0.548156	-3.193501	-0.518932
53	6	0	1.415078	-3.249003	-0.389345
54	6	0	2.648530	-3.334558	-0.274619
55	6	0	4.067399	-3.427328	-0.137136
56	6	0	4.895468	-2.359903	-0.555097
57	6	0	6.294953	-2.430956	-0.420822
58	6	0	6.877010	-3.588985	0.143082
59	6	0	6.062867	-4.654726	0.560310
60	6	0	4.670639	-4.584073	0.426984
61	6	0	-0.929698	0.332305	-1.640945
62	6	0	-3.433429	-0.157009	1.567860
63	6	0	0.449862	0.420378	-1.926471
64	6	0	0.912316	0.649588	-3.235498
65	6	0	-0.000862	0.780460	-4.302068
66	6	0	-1.379482	0.689796	-4.057925
67	6	0	-1.849243	0.476048	-2.741755
68	6	0	-3.379496	-0.330877	2.969378

69	6	0	-4.552305	-0.418348	3.746899
70	6	0	-5.819878	-0.332890	3.138870
71	6	0	-5.914409	-0.160428	1.748948
72	6	0	-4.742160	-0.073057	0.967291
73	6	0	-4.765437	0.126112	-0.493001
74	6	0	-5.884750	0.243217	-1.339200
75	6	0	-5.686939	0.433005	-2.718310
76	6	0	-4.391115	0.509773	-3.255106
77	6	0	-3.279011	0.399576	-2.396137
78	7	0	-3.508753	0.208236	-1.049233
79	78	0	-1.904899	0.045507	0.169377
80	6	0	-0.363001	-0.151708	1.267561
81	6	0	1.907295	-0.453284	2.402630
82	6	0	2.172684	-1.061252	3.655543
83	6	0	2.986413	-0.022158	1.596240
84	6	0	3.487458	-1.247861	4.068845
85	6	0	4.302902	-0.204973	2.017250
86	6	0	4.571615	-0.828536	3.257954
87	7	0	0.609137	-0.306413	1.947088
88	8	0	5.823483	-1.077565	3.760595
89	6	0	6.988615	-0.639621	2.949436
90	1	0	7.860281	-0.931109	3.551833
91	1	0	6.999648	-1.149497	1.972829
92	1	0	6.973643	0.458675	2.803247
93	1	0	1.337663	-1.389104	4.280149
94	1	0	3.721957	-1.728997	5.016889
95	1	0	2.778318	0.455492	0.631533
96	1	0	5.113517	0.084249	1.338278
97	1	0	4.036950	-5.415120	0.744904
98	1	0	6.520280	-5.545644	0.997436

99	1	0	7.960081	-3.652470	0.274377
100	1	0	4.456637	-1.461031	-0.990291
101	1	0	8.928620	-2.409854	-1.280582
102	1	0	10.188043	-0.391270	-2.075362
103	1	0	9.031124	1.813509	-2.181687
104	1	0	4.622272	1.364893	-0.660881
105	1	0	4.217391	5.580624	-1.605239
106	1	0	6.583008	5.594684	-2.414548
107	1	0	7.954260	3.540836	-2.330552
108	1	0	1.170653	0.314484	-1.111104
109	1	0	1.987450	0.732506	-3.425342
110	1	0	0.364151	0.953806	-5.317788
111	1	0	-2.082569	0.794279	-4.891242
112	1	0	-4.238466	0.664592	-4.324410
113	1	0	-6.552371	0.524905	-3.379931
114	1	0	-6.892279	0.186533	-0.924540
115	1	0	-2.402183	-0.402922	3.460685
116	1	0	-4.482520	-0.555419	4.831410
117	1	0	-6.726889	-0.399878	3.744869
118	1	0	-6.903108	-0.093670	1.282026
119	1	0	-6.347866	-3.390855	-0.883633
120	1	0	-4.984539	-3.163191	-2.965042
121	1	0	-5.238219	-3.559776	1.350749
122	1	0	-3.907443	-3.843558	3.186398
123	1	0	-2.273703	-4.195495	5.054605
124	1	0	0.200621	-4.111732	4.552249
125	1	0	0.946835	-3.646933	2.179280
126	1	0	1.250939	-2.944781	-3.053763
127	1	0	0.798495	-2.885850	-5.540869
128	1	0	-1.592718	-2.982202	-6.344249

129	1	0	-3.439522	-3.104045	-4.653847
130	1	0	-5.706572	3.158134	2.098451
131	1	0	-3.889788	2.795263	3.766519
132	1	0	-5.158723	3.668098	-0.288650
133	1	0	-1.993300	2.630870	5.037335
134	1	0	0.200573	2.405679	6.232150
135	1	0	2.342080	2.592668	4.907110
136	1	0	2.200566	3.012079	2.418603
137	1	0	-4.299039	4.230405	-2.339233
138	1	0	-3.156714	4.711083	-4.518666
139	1	0	-0.638019	4.579413	-4.636956
140	1	0	0.650052	3.977303	-2.543992
