Flexible steric bulk of sugar wingtip substituents on bis(N-heterocyclic carbene) ligands of diplatinum complexes via chair–twist-boat conformational changes

Shuhei Nomura,[a] Itsuki Kobayashi,[a] Matsumi Doe,[b] Rika Tanaka,[b] Tamaki Nagasawa[b] and Takanori Nishioka*[a]

[a] *Department of Chemistry, Graduate School of Science, Osaka Metropolitan University, Osaka 558-8585, Japan. E-mail: nishioka@omu.ac.jp.*

[b] *Analytical Research Centre, Osaka Metropolitan University, Osaka 558-8585, Japan.*

Supplementary Information

1. NMR spectroscopic data and electrospray mass spectral data of the platinum complexes bearing bisNHC ligands with AcGlc groups.
2. Reactions of diplatinum complexes [**1**]$(PF_6)_2$ and [**2**]$(PF_6)_2$ with 2-FPhMgBr confirmed by ^{19}F NMR spectroscopy and electrospray mass spectrometry.
3. X-ray crystallography of [**1**]$(PF_6)_2$ and [**2**]$(PF_6)_2$.
4. DFT calculations of **4c**, **2c-2tb**, **2tb-2c** and **4tb** isomers of $[\mathbf{1}]^{2+}$ and $[\mathbf{2}]^{2+}$.

1. NMR spectra and electrospray mass spectral data of the platinum complexes bearing bisNHC ligands with AcGlc groups.

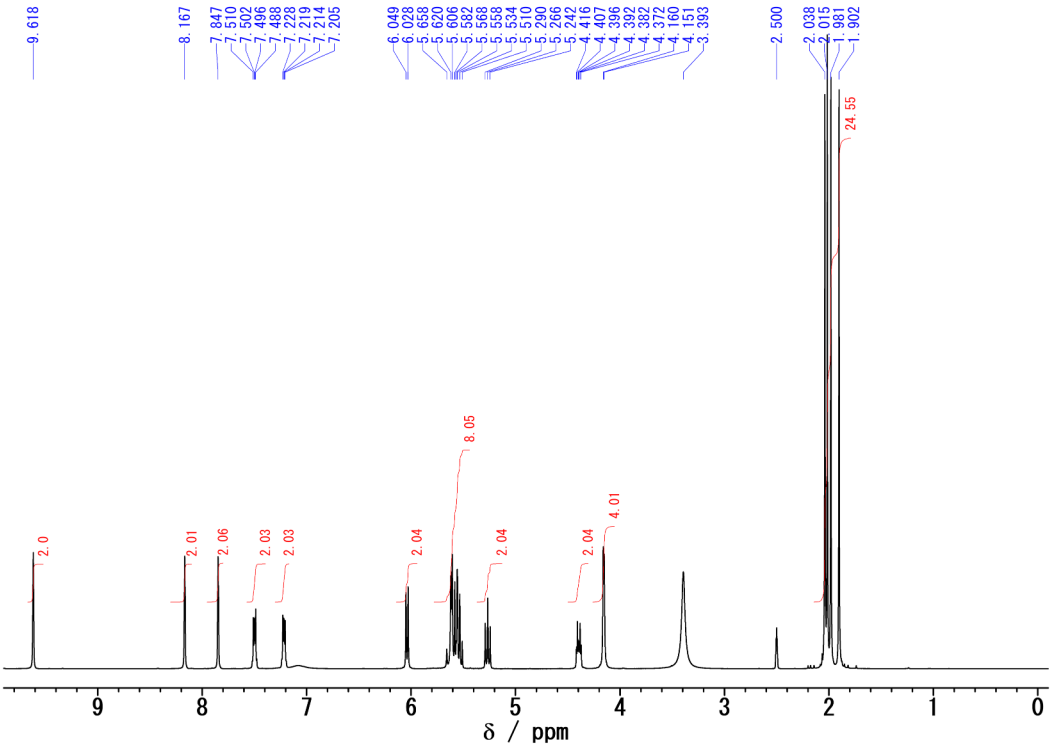

Fig. S1 ^{1}H NMR spectrum of [(bisNHC-C4)H$_2$](PF$_6$)$_2$ (DMSO-d_6, 400 MHz, 293 K).

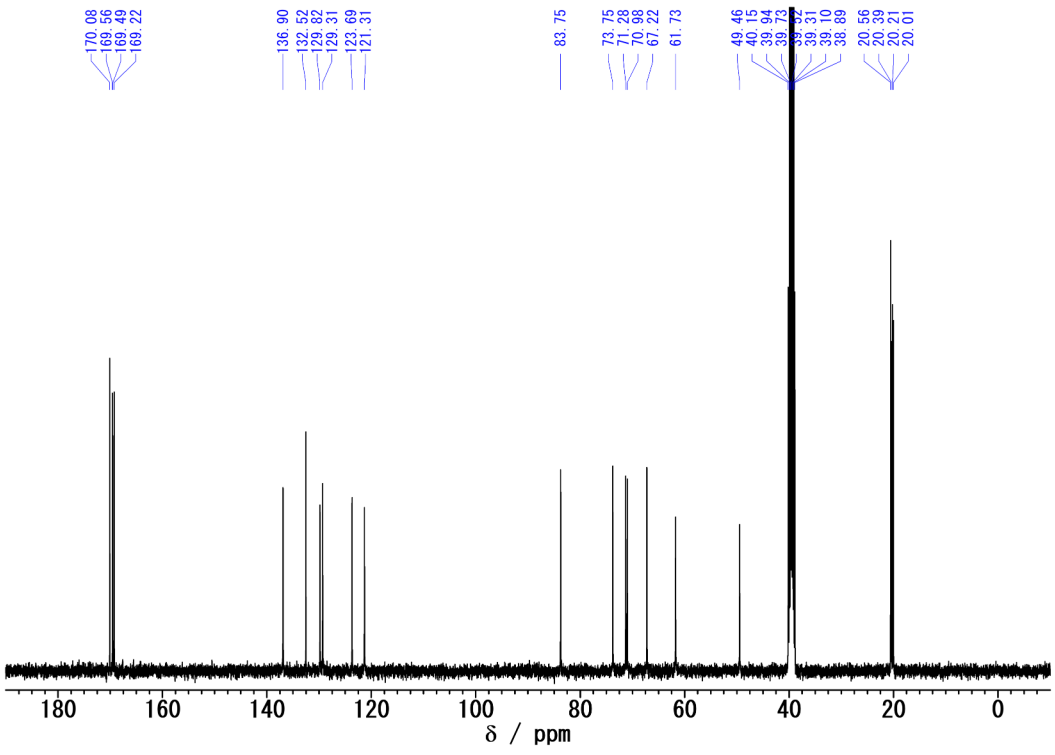

Fig. S2 ^{13}C NMR spectrum of [(bisNHC-C4)H$_2$](PF$_6$)$_2$ (DMSO-d_6, 100 MHz, 293 K).

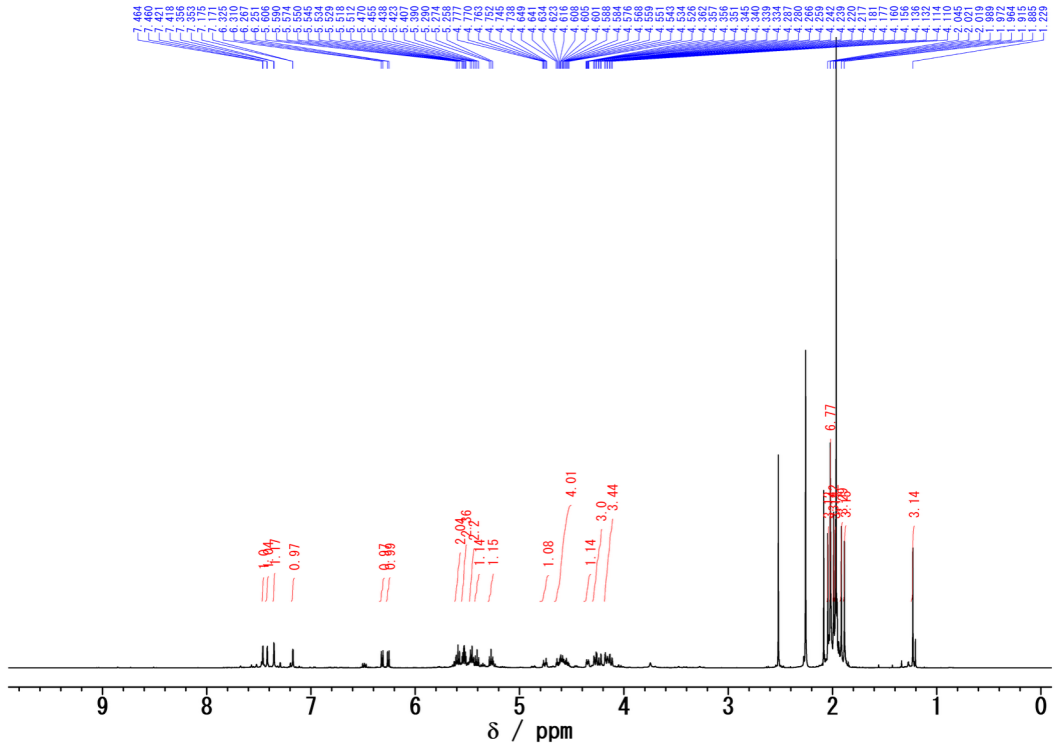

Fig. S3 ^{1}H NMR spectrum of [Pt(bisNHC-C2)(NCMe)$_2$](PF$_6$)$_2$ ([**4**](PF$_6$)$_2$) (CD$_3$CN, 600 MHz).

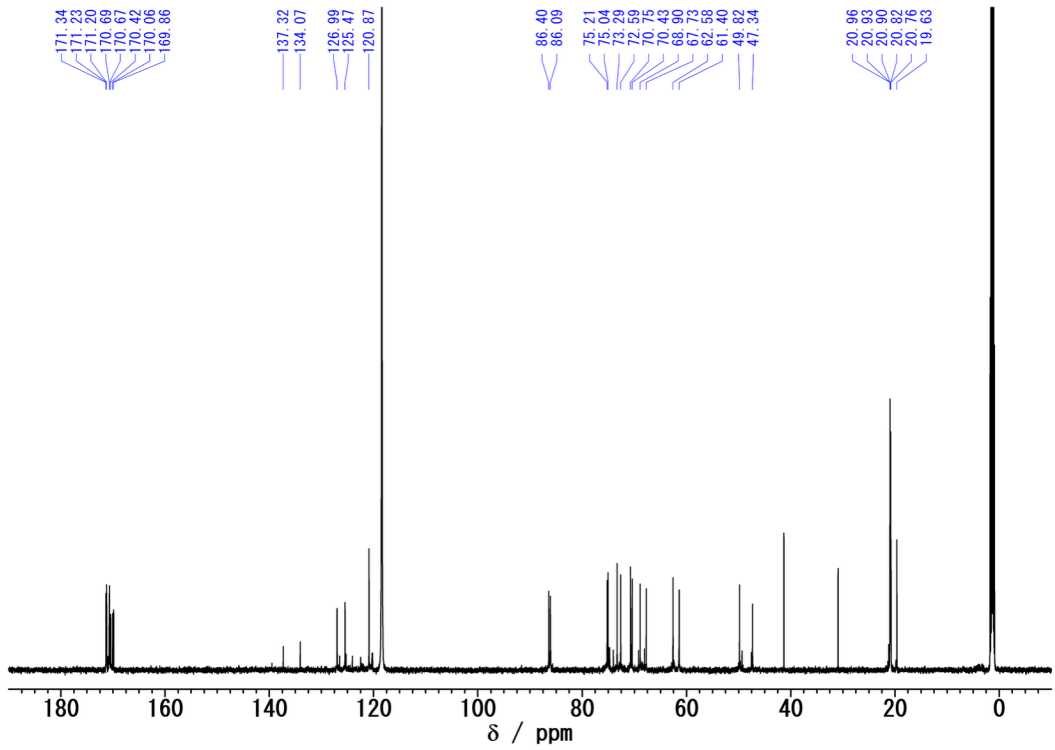

Fig. S4 ^{13}C NMR spectrum of [Pt(bisNHC-C2)(NCMe)$_2$](PF$_6$)$_2$ ([**4**](PF$_6$)$_2$) (CD$_3$CN, 150 MHz).

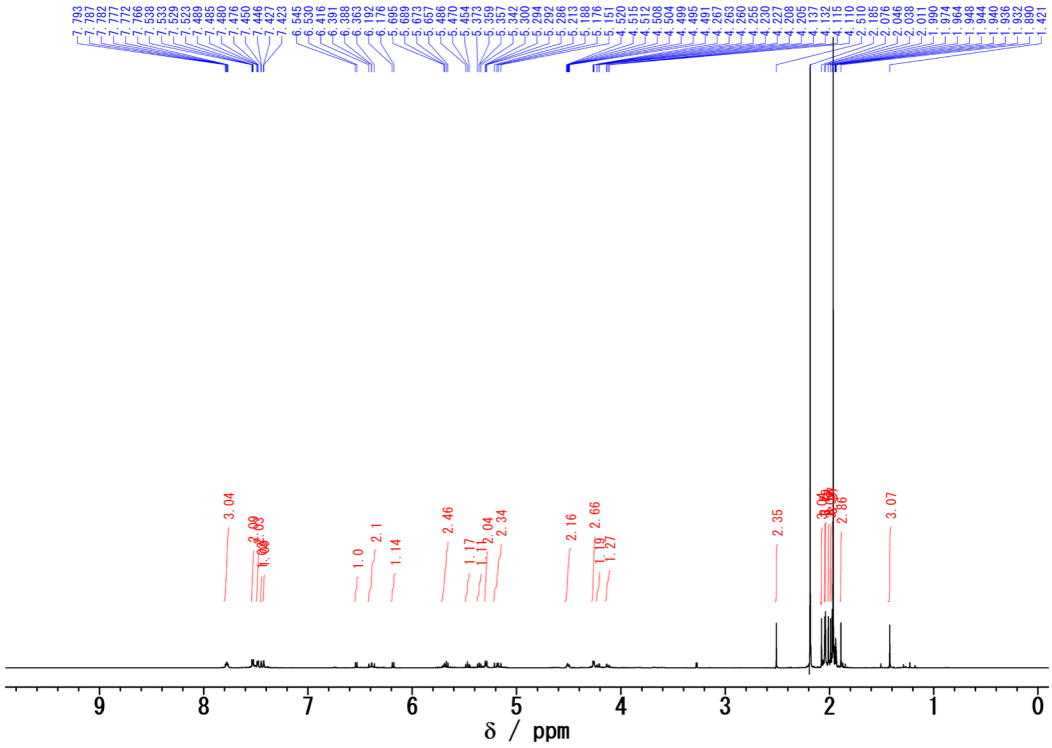

Fig. S5 ^{1}H NMR spectrum of [Pt(bisNHC-C4)(NCMe)$_2$](PF$_6$)$_2$ ([**5**](PF$_6$)$_2$) (CD$_3$CN, 600 MHz).

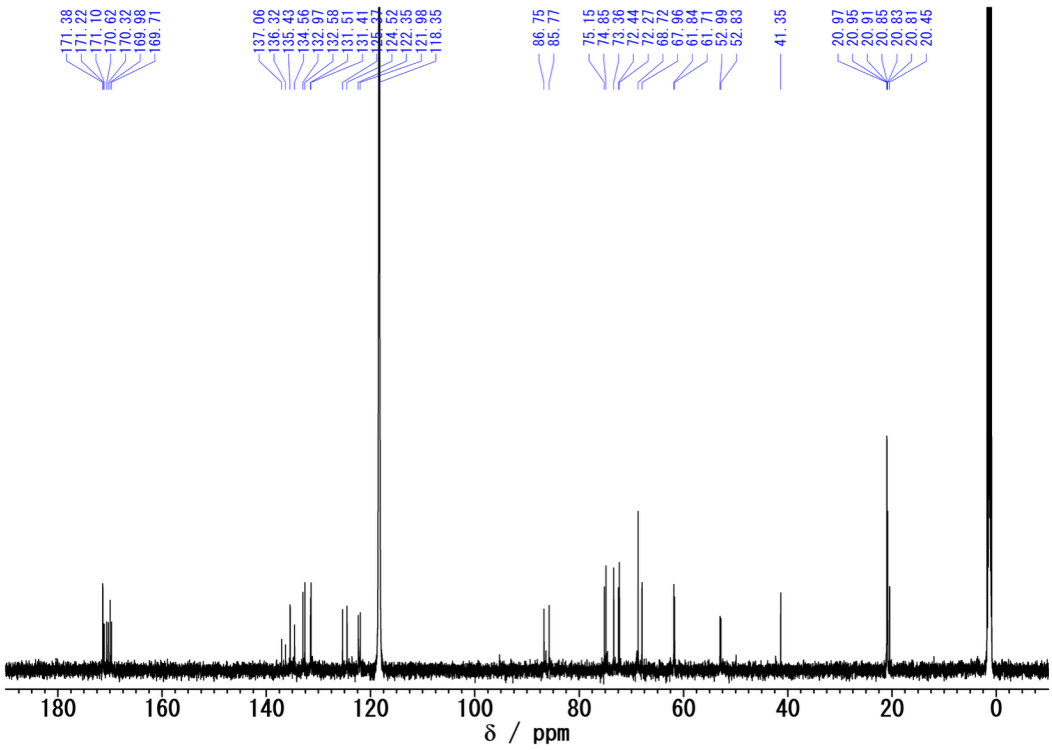

Fig. S6 ^{13}C NMR spectrum of [Pt(bisNHC-C4)(NCMe)$_2$](PF$_6$)$_2$ ([**5**](PF$_6$)$_2$) (CD$_3$CN, 150 MHz).

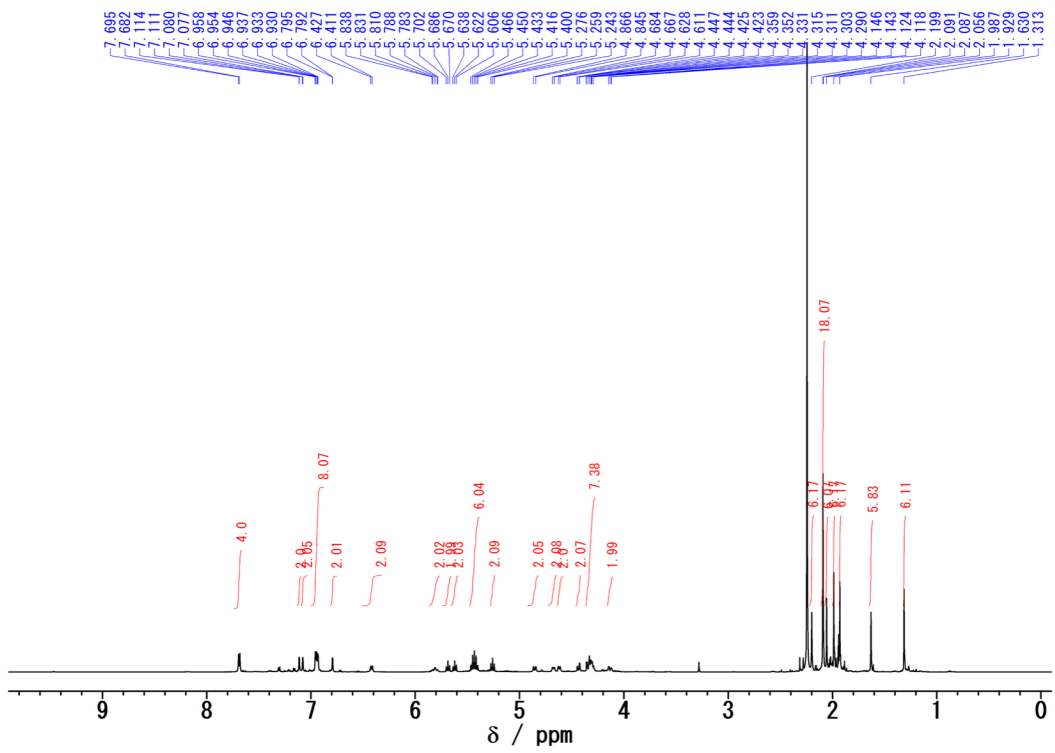

Fig. S7 ^{1}H NMR spectrum of [{Pt(bisNHC-C2)}$_2${μ-(S-*p*-tol)}$_2$](PF$_6$)$_2$ ([**1**](PF$_6$)$_2$) (CD$_3$CN, 600 MHz).

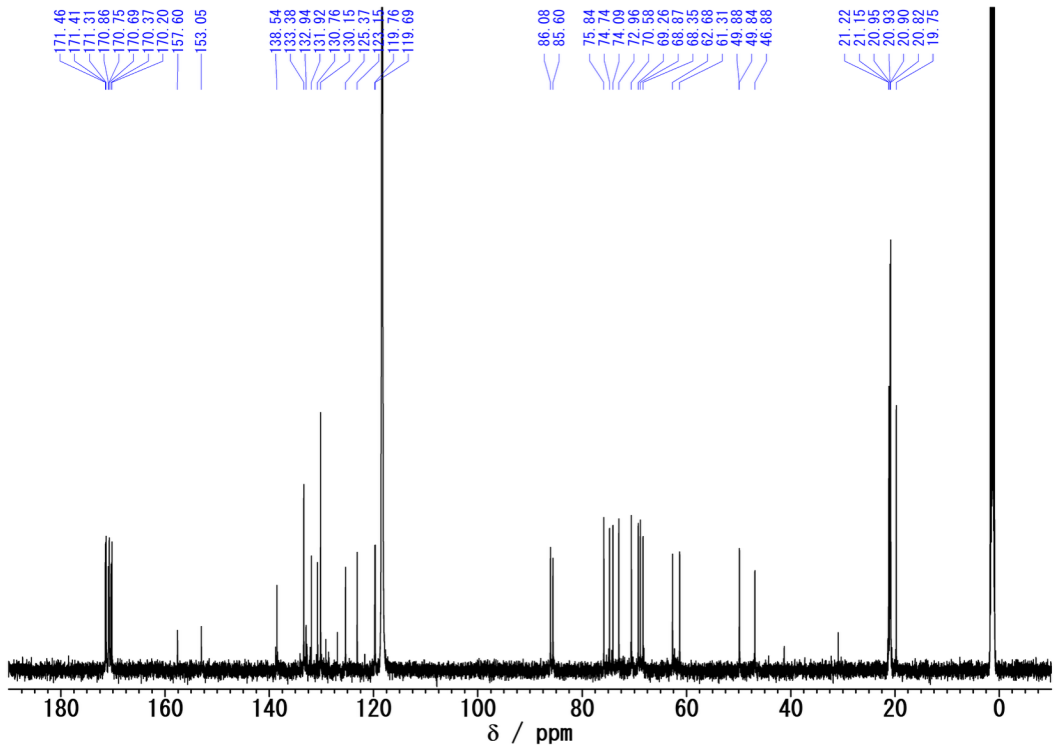

Fig. S8 ^{13}C NMR spectrum of [{Pt(bisNHC-C2)}$_2${μ-(S-*p*-tol)}$_2$](PF$_6$)$_2$ ([**1**](PF$_6$)$_2$) (CD$_3$CN, 150 MHz).

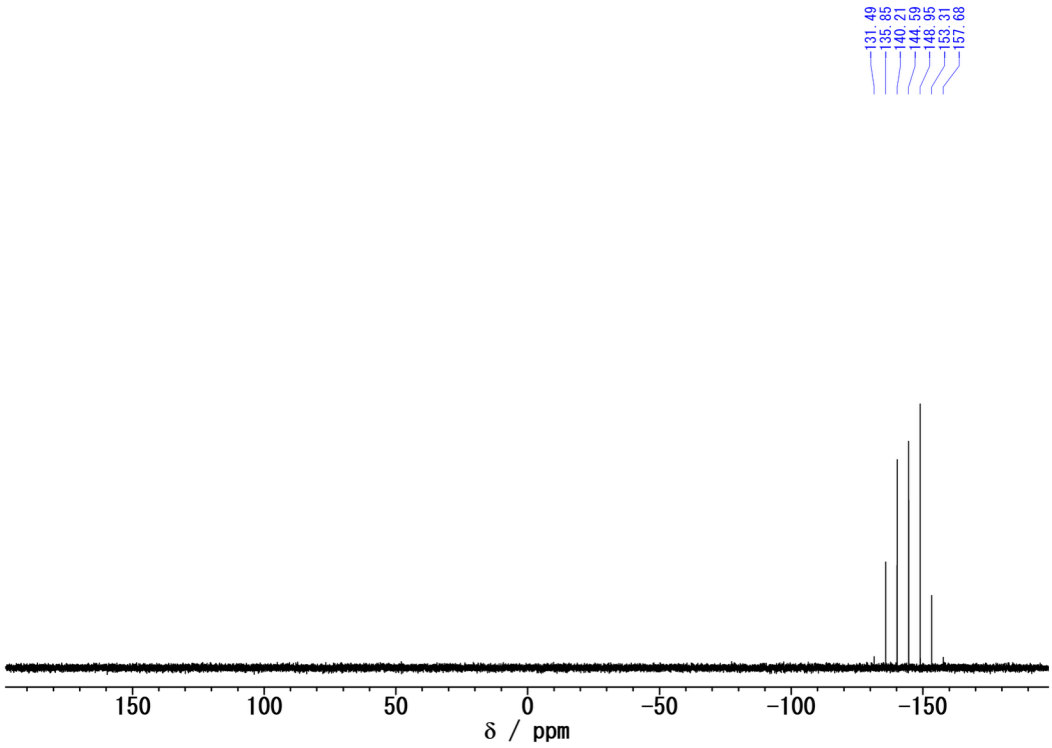

Fig. S9 ^{31}P NMR spectrum of [{Pt(bisNHC-C2)}$_2${μ-(S-*p*-tol)}$_2$](PF$_6$)$_2$ ([**1**](PF$_6$)$_2$) (CD$_3$CN, 162 MHz).

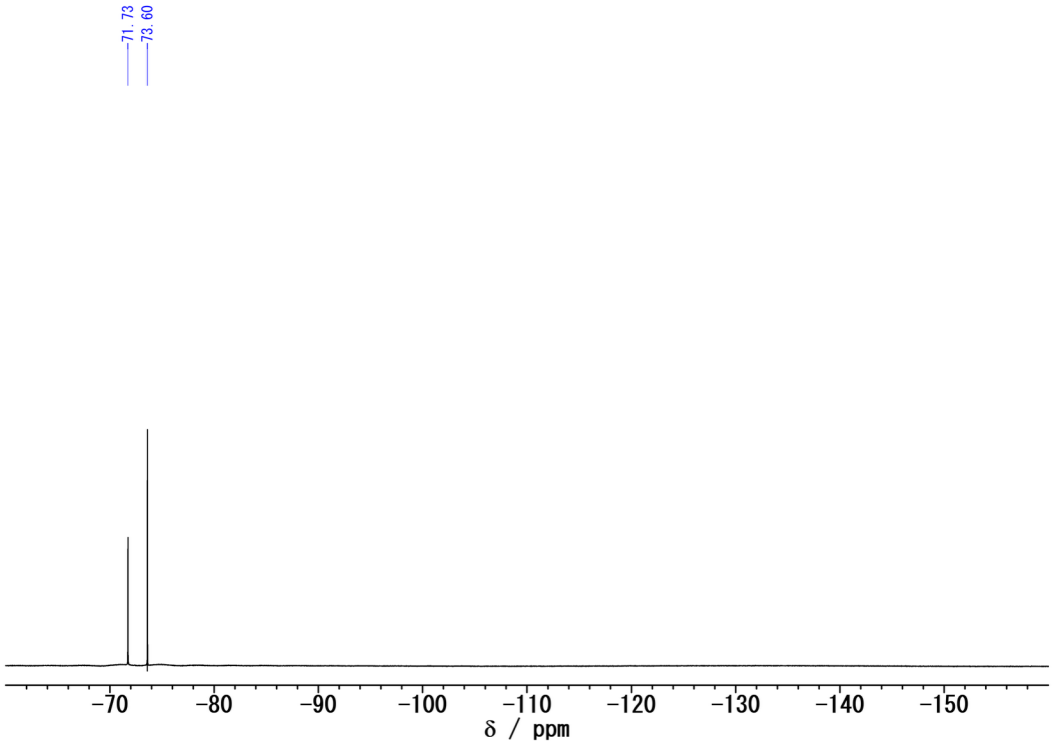

Fig. S10 ^{19}F NMR spectrum of [{Pt(bisNHC-C2)}$_2${μ-(S-*p*-tol)}$_2$](PF$_6$)$_2$ ([**1**](PF$_6$)$_2$) (CD$_3$CN, 376.5 MHz).

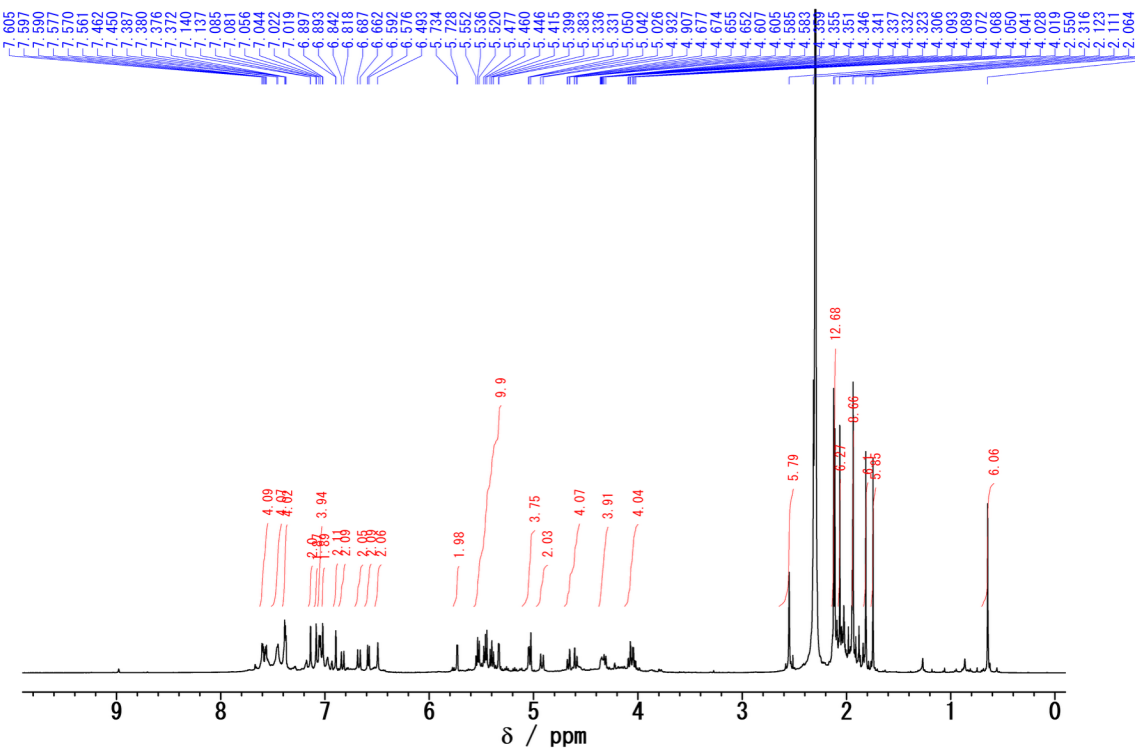

Fig. S11 ^{1}H NMR spectrum of [{Pt(bisNHC-C4)}$_2${μ-(S-*p*-tol)}$_2$](PF$_6$)$_2$ ([**2**](PF$_6$)$_2$) (CD$_3$CN, 600 MHz).

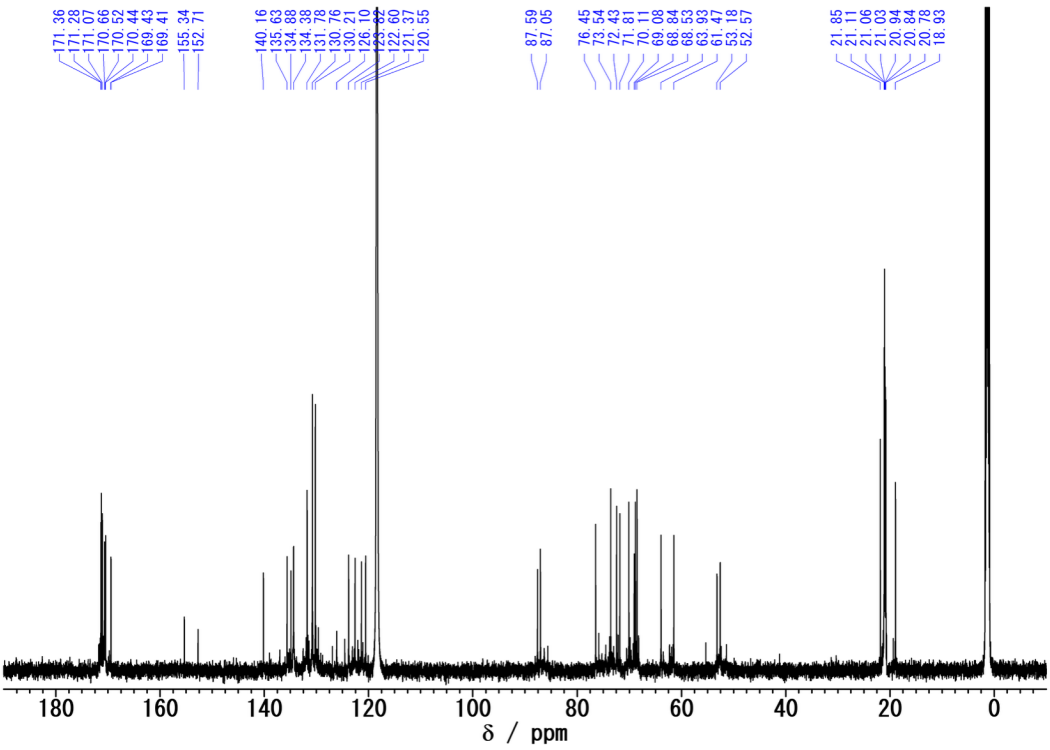

Fig. S12 ^{13}C NMR spectrum of [{Pt(bisNHC-C4)}$_2${μ-(S-*p*-tol)}$_2$](PF$_6$)$_2$ ([**2**](PF$_6$)$_2$) (CD$_3$CN, 150 MHz).

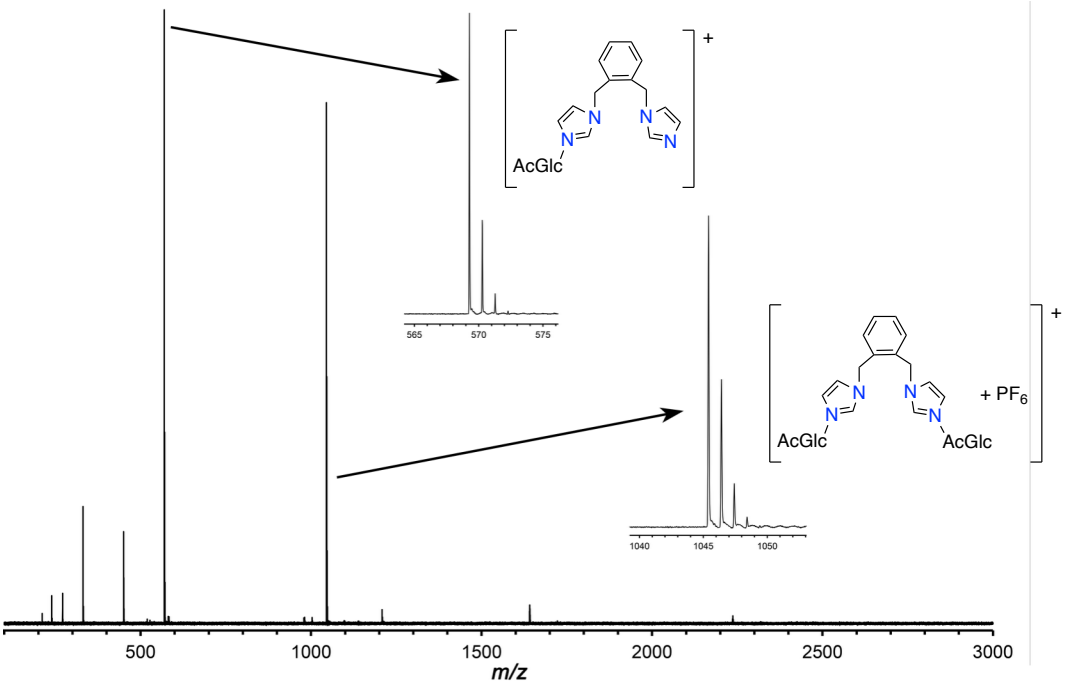

Fig. S13 ESI-mass spectrum of $[(bisNHC\text{-}C4)H_2](PF_6)_2$ in MeCN.

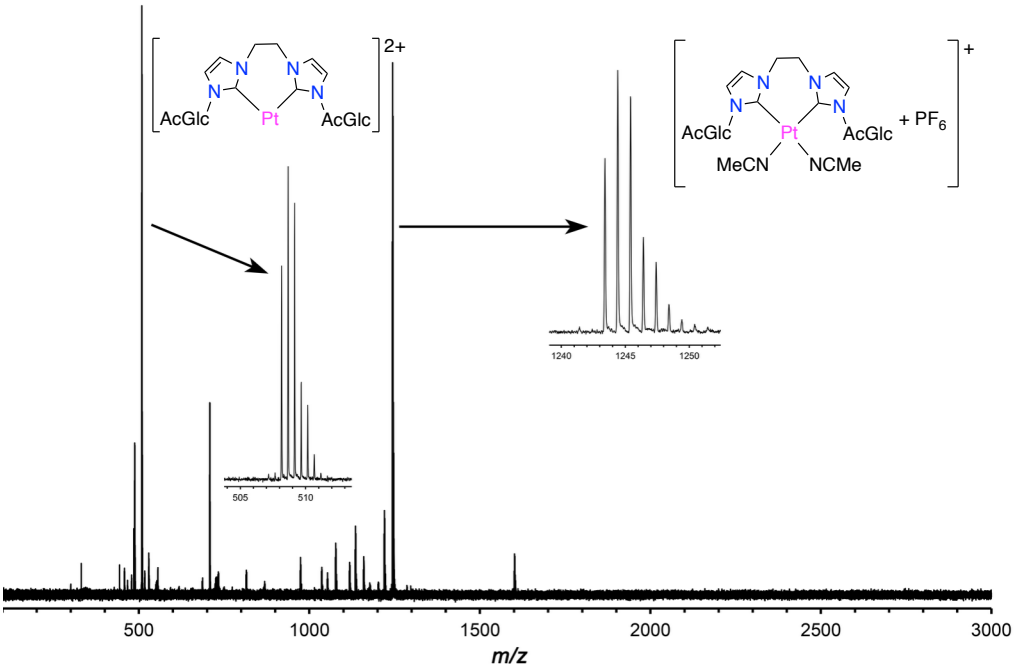

Fig. S14 ESI-mass spectrum of [Pt(bisNHC-C2)(NCMe)$_2$](PF$_6$)$_2$ ([**4**](PF$_6$)$_2$) in MeCN.

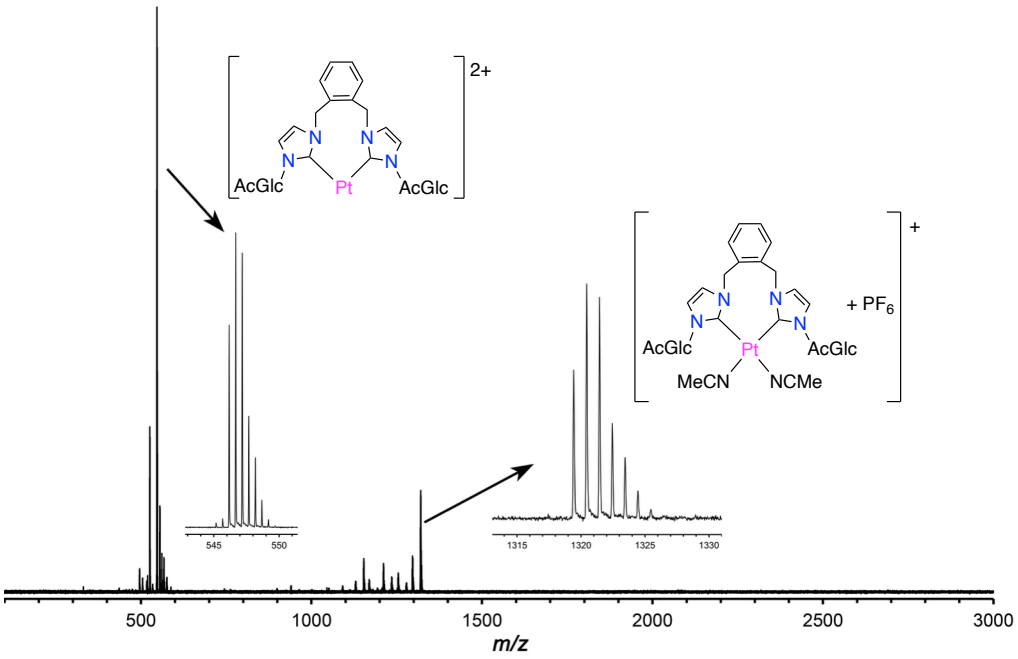

Fig. S15 ESI-mass spectrum of [Pt(bisNHC-C4)(NCMe)$_2$](PF$_6$)$_2$ ([**5**](PF$_6$)$_2$) in MeCN.

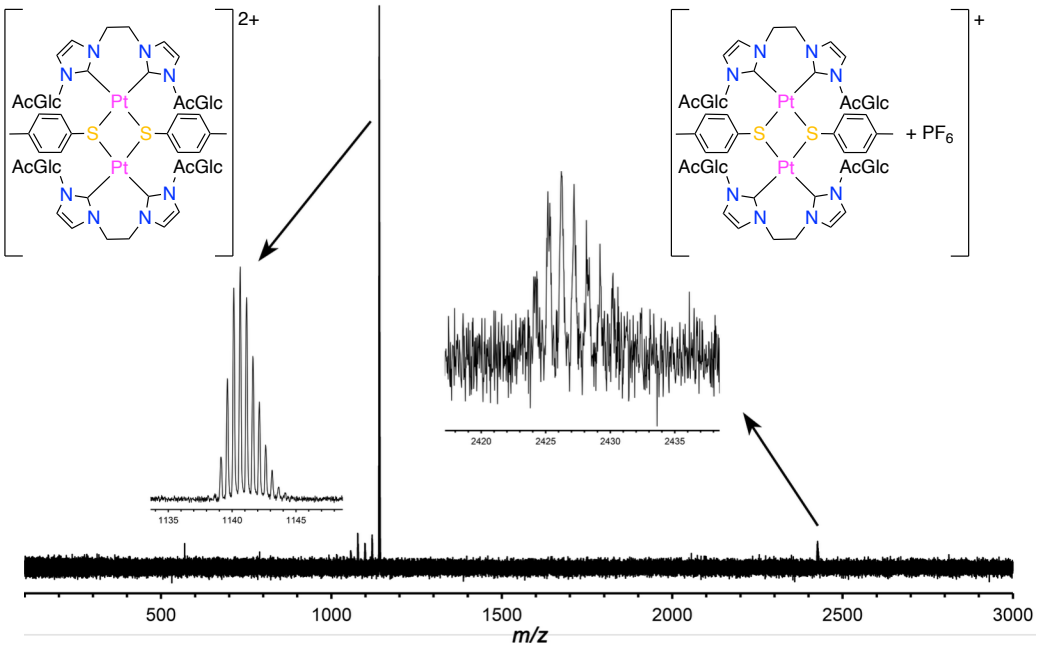

Fig. S16 ESI-mass spectrum of diplatinum bisNHC-C2 complex [**1**]$(PF_6)_2$ in MeCN.

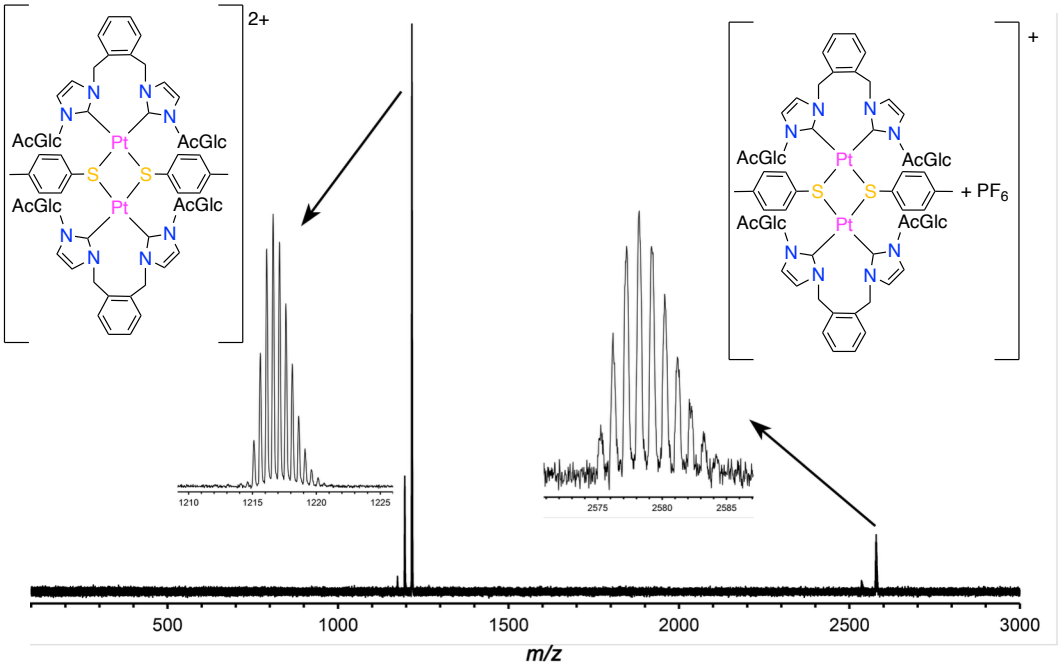

Fig. S17 ESI-mass spectrum of diplatinum bisNHC-C4 complex [**2**]$(PF_6)_2$ in MeCN.

2. Reactions of diplatinum complexes [1](PF$_6$)$_2$ and [2](PF$_6$)$_2$ with 2-FPhMgBr confirmed by ^{19}F NMR spectroscopy and electrospray mass spectrometry.

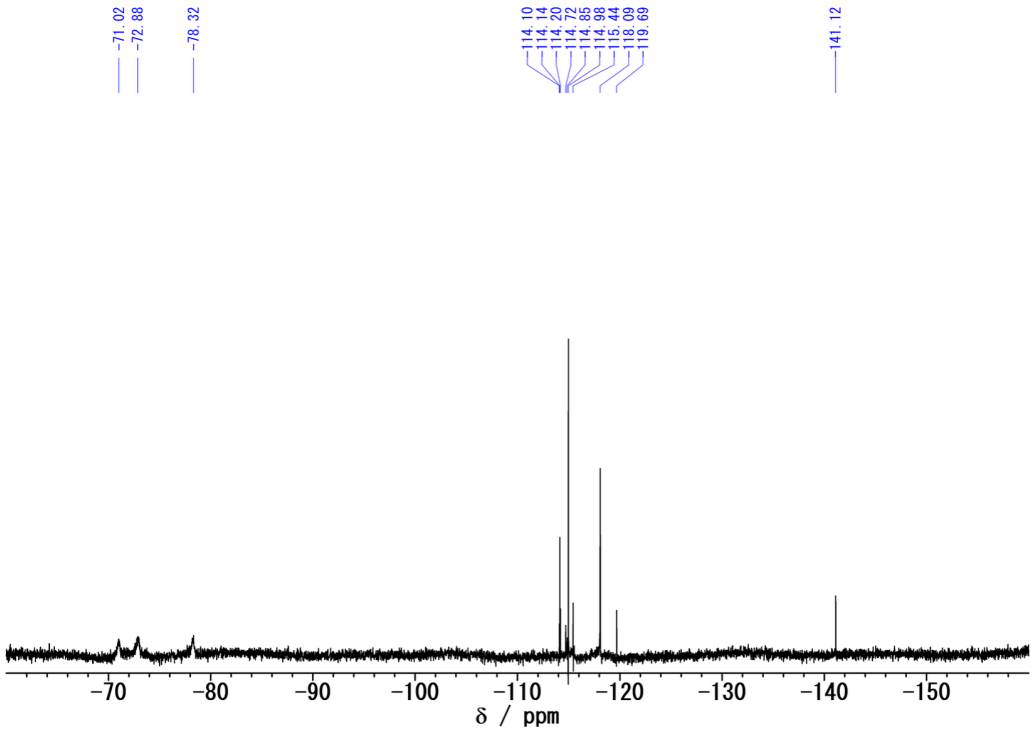

Fig. S18 ^{19}F NMR spectrum of products of reaction of [**1**](PF$_6$)$_2$ with 2-FPhMgBr (CDCl$_3$, 376.5 MHz).

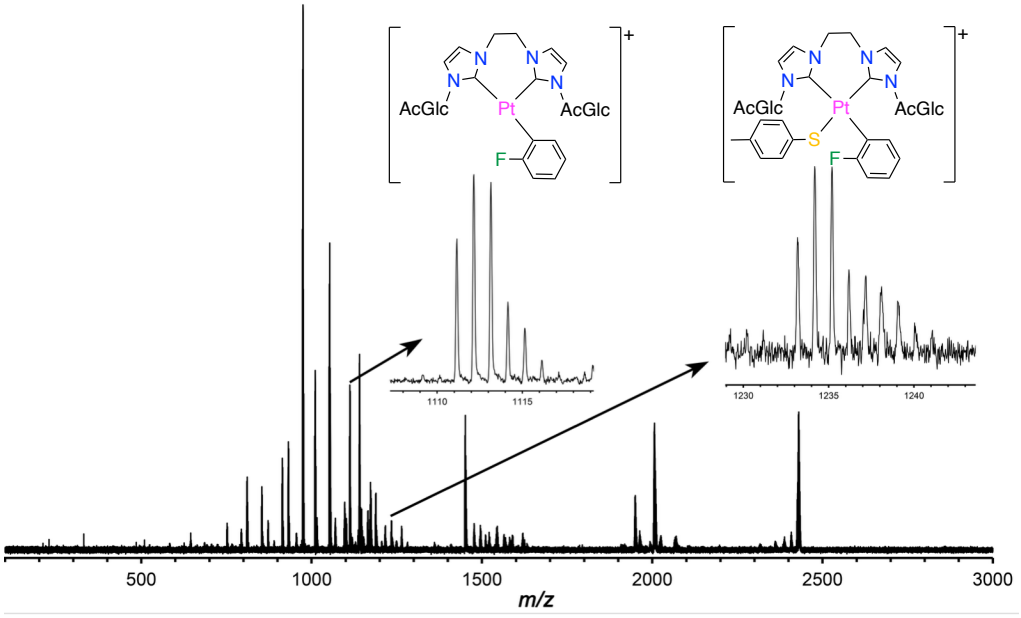

Fig. S19 ESI-mass spectrum of products of reaction of [**1**](PF$_6$)$_2$ with 2-FPhMgBr (MeCN).

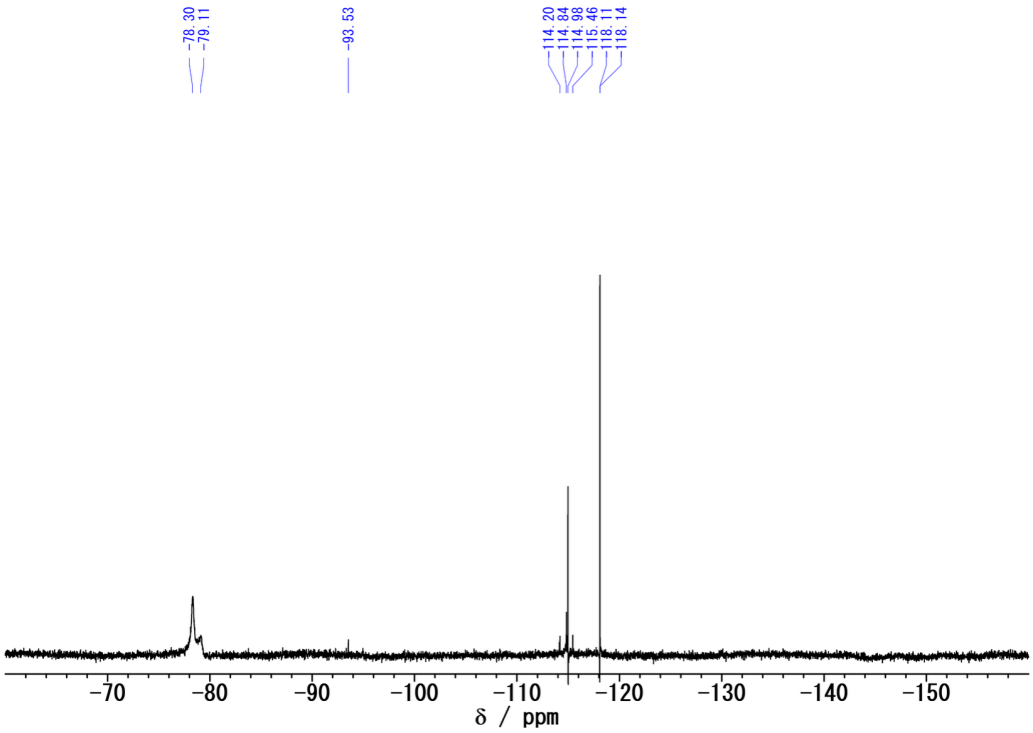

Fig. S20 ^{19}F NMR spectrum of products of reaction of [**2**](PF$_6$)$_2$ with 2-FPhMgBr (CDCl$_3$, 376.5 MHz).

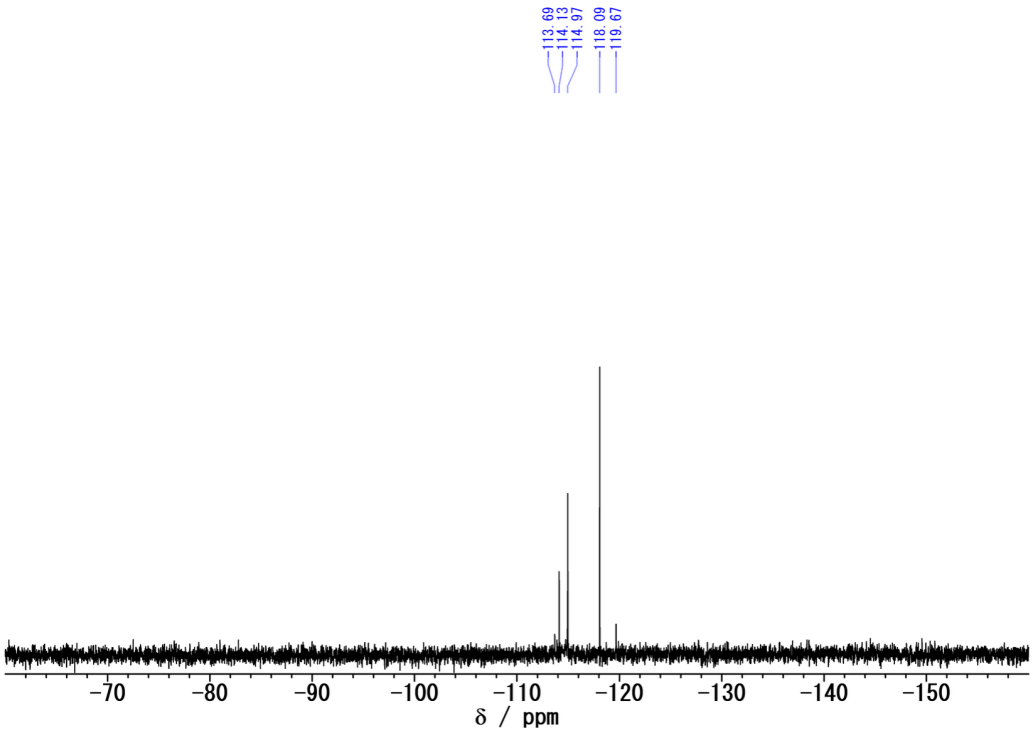

Fig. S21 ^{19}F NMR spectrum of decomposition products of 2-FPhMgBr (CDCl$_3$, 376.5 MHz).

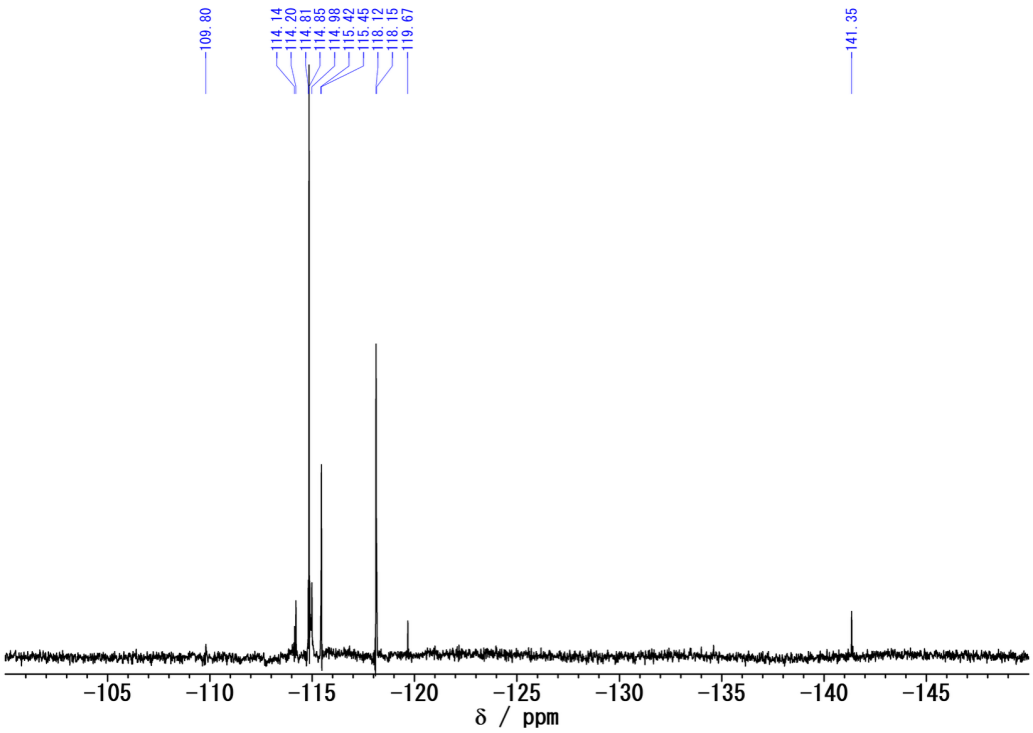

Fig. S22 ^{19}F NMR spectrum of decomposition products of reaction mixture of [**1**]$(PF_6)_2$ with 2-FPhMgBr ($CDCl_3$, 376.5 MHz).

3. X-ray crystallography.

Table S1. Crystallographic data of ethylene-bridged bisNHC-C2 complex [**1**]$(PF_6)_2$ (CCDC 2518861).

Formula	$C_{86}H_{106}F_{12}N_8O_{36}P_2Pt_2S_2$ [+ solvent]
M_w	2572.02
Crystal description	block, colourless
Crystal size/mm	0.380 × 0.080 × 0.060
Crystal system	*orthorhombic*
Space Group	$P2_12_12$
a/ Å	22.5854(4)
b/ Å	22.3926(5)
c/ Å	11.3900(2)
α/°	90
β/°	90
γ/°	90
V/Å^3	5760.45(19)
Z	2
F(000)	2584
ρ_{calcd}/g cm^{-1}	1.483
μ/mm^{-1}	2.586
Total reflections	59636
Unique reflections (R_{int})	13226 (0.0635)
Scan range θ/°	2.199 to 27.500
Completeness	0.998
Index ranges	$-27 \leq h \leq 29$
	$-29 \leq k \leq 28$
	$-14 \leq l \leq 14$
Data/restrains/para.	13226/0/703
*R*1 [$I>2\sigma(I)$], *wR*2 (all data)	0.0400, 0.1045
GOF on F^2	1.081
Flack parameter	–0.016(3)
Max./min. ρ/eÅ^{-3}	1.642/–1.012
Min./max. *T*	0.62546/1.00000

Table S2. Crystallographic data of *o*-xylene-bridged bisNHC-C4 complex [**2**](PF$_6$)$_2$ (CCDC 2518862).

Formula	$C_{98}H_{114}F_{12}N_8O_{36}P_2Pt_2S_2$ [+ solvent]
M_w	2984.14
Crystal description	block, colourless
Crystal size/mm	0.350 × 0.150 × 0.050
Crystal system	*monoclinic*
Space Group	$P2_1$
a/ Å	13.7862(2)
b/ Å	32.9435(5)
c/ Å	13.9227(2)
α/°	90
β/°	91.5185(12)
γ/°	90
V/Å^3	6320.99(16)
Z	2
F(000)	3012
ρ_{calcd}/g cm^{-1}	1.568
μ/mm^{-1}	2.453
Total reflections	69528
Unique reflections (R_{int})	27985 (0.0352)
Scan range θ/°	2.362 to 27.498
Completeness	0.987
Index ranges	$-17 \leq h \leq 17$
	$-42 \leq k \leq 42$
	$-18 \leq l \leq 18$
Data/restrains/para.	27985/85/1592
*R*1 [*I*>2σ(*I*)], *wR*2 (all data)	0.0525, 0.1344
GOF on F^2	1.074
Flack parameter	0.013(3)
Max./min. ρ/eÅ^{-3}	3.998/–1.342
Min./max. *T*	0.61335/1.00000

4. DFT calculations.

Table S3. Optimised atomic coordinates of **4c** isomer of complex $[\mathbf{1}]^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	0.418582	1.810674	2.141094
2	C	2.121036	2.810212	2.510028
3	N	2.382272	3.330521	3.749130
4	C	3.645179	3.952337	3.776127
5	H	4.051244	4.421473	4.657112
6	C	4.172685	3.820947	2.522070
7	H	5.105544	4.175097	2.119708
8	N	3.221244	3.127903	1.748529
9	C	1.428391	3.200113	4.858966
10	C	0.301285	4.243818	4.828443
11	C	–0.577633	3.540116	2.473991
12	N	–0.489686	4.364632	3.574858
13	C	–1.337010	5.483534	3.422708
14	H	–1.433687	6.242692	4.181651
15	C	–1.949780	5.367311	2.212908
16	H	–2.689042	5.996923	1.747516
17	N	–1.481212	4.174519	1.635128
18	O	4.376942	1.630968	0.366676
19	C	3.401636	2.711492	0.362735
20	H	2.427109	2.347701	0.008074
21	C	3.925386	3.825989	–0.570451
22	H	4.907342	4.174433	–0.232672
23	C	4.030933	3.247103	–1.992229
24	H	3.044417	2.937014	–2.360409
25	C	4.984714	2.041977	–2.002379
26	H	6.018035	2.346121	–1.809629
27	C	4.527314	0.993090	–0.958220
28	H	3.546452	0.593326	–1.265094
29	O	2.987132	4.945768	–0.587485
30	C	3.402480	6.153760	0.018919
31	O	4.464872	6.228060	0.647471
32	C	2.404001	7.248357	–0.217022
33	H	1.388301	6.890669	–0.015424
34	H	2.443238	7.548677	–1.271160
35	H	2.643274	8.105796	0.414729
36	O	4.549696	4.293479	–2.866457
37	C	3.790385	4.637098	–4.001982
38	O	2.742344	4.041902	–4.288485
39	C	4.398512	5.797690	–4.734810
40	H	5.447206	5.934773	–4.465383
41	H	3.830486	6.697613	–4.465335
42	H	4.295565	5.649567	–5.813680
43	O	4.879123	1.425650	–3.327437
44	C	6.059156	1.054268	–4.001598
45	O	7.179702	1.233065	–3.510324
46	C	5.730516	0.405345	–5.316280
47	H	4.893989	0.915066	–5.802344
48	H	5.438938	–0.633503	–5.115677
49	H	6.611392	0.411855	–5.961632
50	C	5.479668	–0.176390	–0.797694
51	H	5.174640	–0.805203	0.044240
52	H	5.485033	–0.783955	–1.706750
53	O	6.828809	0.364917	–0.561330
54	C	7.892751	–0.500812	–0.760052
55	O	7.715318	–1.724352	–0.914318

56	C	9.205186	0.230388	–0.789065
57	H	10.032622	–0.476286	–0.703558
58	H	9.253999	0.976274	0.010327
59	H	9.276457	0.763503	–1.745836
60	O	–0.832042	4.591286	–0.574449
61	C	–1.738768	3.791021	0.247806
62	H	–1.510411	2.722880	0.144934
63	C	–3.169353	4.102399	–0.236529
64	H	–3.354216	5.179885	–0.172444
65	C	–3.328550	3.663354	–1.702783
66	H	–3.312393	2.570664	–1.796621
67	C	–2.244309	4.284449	–2.605159
68	H	–2.499274	5.326190	–2.817545
69	C	–0.827898	4.177309	–1.993377
70	H	–0.499753	3.126391	–2.047517
71	O	–4.171563	3.388453	0.555275
72	C	–5.115358	4.173850	1.259115
73	O	–4.961287	5.392940	1.399972
74	C	–6.251172	3.334505	1.763603
75	H	–5.867573	2.465151	2.308633
76	H	–6.837061	2.967556	0.911047
77	H	–6.889443	3.934971	2.414459
78	O	–4.651864	4.172383	–2.092407
79	C	–5.471027	3.408620	–2.921178
80	O	–5.104805	2.302871	–3.360464
81	C	–6.799221	4.068235	–3.145583
82	H	–6.733311	5.147296	–2.995776
83	H	–7.514759	3.643548	–2.428832
84	H	–7.156525	3.845175	–4.154382
85	O	–2.144648	3.527665	–3.862435
86	C	–2.793600	4.023014	–5.007657
87	O	–3.470859	5.055608	–4.985764
88	C	–2.537754	3.120342	–6.184042
89	H	–2.962428	2.130013	–5.982759
90	H	–1.460789	2.994181	–6.339825
91	H	–2.996414	3.542899	–7.079675
92	C	0.203128	5.033245	–2.715264
93	H	1.083257	5.173593	–2.083485
94	H	0.515051	4.568769	–3.653888
95	O	–0.418653	6.341033	–3.017851
96	C	0.402384	7.369897	–3.448693
97	O	1.641079	7.258845	–3.481978
98	C	–0.399599	8.580061	–3.851915
99	H	0.269520	9.419644	–4.048092
100	H	–1.118214	8.843300	–3.068679
101	H	–0.975234	8.355372	–4.758004
102	Pt	–0.418686	–1.810614	2.140997
103	C	–2.121111	–2.810200	2.509981
104	N	–2.382396	–3.330446	3.749098
105	C	–3.645270	–3.952326	3.776063
106	H	–4.051372	–4.421412	4.657057
107	C	–4.172738	–3.820990	2.521984
108	H	–5.105575	–4.175183	2.119610
109	N	–3.221268	–3.127983	1.748442
110	C	–1.428540	–3.199934	4.858956
111	C	–0.301272	–4.243576	4.828550
112	C	0.577544	–3.540039	2.474018
113	N	0.489642	–4.364484	3.574947
114	C	1.336975	–5.483385	3.422831
115	H	1.433674	–6.242507	4.181808

116	C	1.949720	–5.367220	2.213007
117	H	2.688988	–5.996832	1.747624
118	N	1.481114	–4.174468	1.635179
119	O	–4.376886	–1.631078	0.366522
120	C	–3.401602	–2.711613	0.362640
121	H	–2.427056	–2.347844	0.008005
122	C	–3.925333	–3.826093	–0.570578
123	H	–4.907354	–4.174463	–0.232912
124	C	–4.030661	–3.247181	–1.992361
125	H	–3.044080	–2.937117	–2.360387
126	C	–4.984411	–2.042033	–2.002608
127	H	–6.017759	–2.346157	–1.809980
128	C	–4.527144	–0.993158	–0.958368
129	H	–3.546262	–0.593349	–1.265113
130	O	–2.987149	–4.945937	–0.587504
131	C	–3.402663	–6.153912	0.018816
132	O	–4.465109	–6.228131	0.647287
133	C	–2.404086	–7.248503	–0.216759
134	H	–1.388425	–6.890708	–0.015162
135	H	–2.443227	–7.549095	–1.270823
136	H	–2.643366	–8.105803	0.415179
137	O	–4.549323	–4.293524	–2.866688
138	C	–3.789832	–4.637154	–4.002089
139	O	–2.741664	–4.042063	–4.288348
140	C	–4.398137	–5.797416	–4.735293
141	H	–5.446976	–5.934145	–4.466249
142	H	–3.830547	–6.697588	–4.465739
143	H	–4.294752	–5.649183	–5.814105
144	O	–4.878658	–1.425685	–3.327647
145	C	–6.058614	–1.054269	–4.001932
146	O	–7.179214	–1.233007	–3.510761
147	C	–5.729805	–0.405147	–5.316473
148	H	–4.893219	–0.914801	–5.802506
149	H	–5.438241	0.633667	–5.115671
150	H	–6.610598	–0.411549	–5.961938
151	C	–5.479557	0.176280	–0.797860
152	H	–5.174616	0.805060	0.044130
153	H	–5.484889	0.783897	–1.706882
154	O	–6.828691	–0.365101	–0.561620
155	C	–7.892651	0.500623	–0.760246
156	O	–7.715269	1.724220	–0.914126
157	C	–9.205083	–0.230587	–0.789248
158	H	–10.032516	0.476038	–0.703301
159	H	–9.253716	–0.976784	0.009862
160	H	–9.276538	–0.763327	–1.746214
161	O	0.831987	–4.591365	–0.574398
162	C	1.738640	–3.791002	0.247841
163	H	1.510195	–2.722884	0.144932
164	C	3.169259	–4.102282	–0.236440
165	H	3.354219	–5.179748	–0.172297
166	C	3.328470	–3.663293	–1.702710
167	H	3.312220	–2.570607	–1.796598
168	C	2.244302	–4.284524	–2.605078
169	H	2.499340	–5.326261	–2.817395
170	C	0.827867	–4.177445	–1.993344
171	H	0.499656	–3.126549	–2.047543
172	O	4.171372	–3.388206	0.555374
173	C	5.115152	–4.173480	1.259370
174	O	4.961041	–5.392532	1.400515
175	C	6.250857	–3.334012	1.763893

176	H	5.867154	–2.464462	2.308534
177	H	6.836969	–2.967360	0.911358
178	H	6.888953	–3.934285	2.415096
179	O	4.651844	–4.172224	–2.092254
180	C	5.471013	–3.408387	–2.920958
181	O	5.104749	–2.302654	–3.360243
182	C	6.799247	–4.067932	–3.145313
183	H	6.733320	–5.147034	–2.995797
184	H	7.514647	–3.643431	–2.428313
185	H	7.156730	–3.844599	–4.153986
186	O	2.144630	–3.527824	–3.862402
187	C	2.793576	–4.023252	–5.007592
188	O	3.470764	–5.055894	–4.985651
189	C	2.537676	–3.120698	–6.184052
190	H	2.962131	–2.130271	–5.982789
191	H	1.460699	–2.994761	–6.339949
192	H	2.996496	–3.543225	–7.079617
193	C	–0.203081	–5.033491	–2.715216
194	H	–1.083208	–5.173856	–2.083441
195	H	–0.515025	–4.569096	–3.653876
196	O	0.418800	–6.341254	–3.017691
197	C	–0.402173	–7.370227	–3.448398
198	O	–1.640878	–7.259286	–3.481596
199	C	0.399892	–8.580411	–3.851402
200	H	–0.269251	–9.419740	–4.048567
201	H	1.117629	–8.844195	–3.067530
202	H	0.976537	–8.355476	–4.756779
203	S	1.608024	–0.372207	1.779219
204	S	–1.608118	0.372269	1.779208
205	C	4.870762	–0.272930	4.325468
206	C	4.038629	–0.181543	3.194034
207	C	2.676041	–0.518045	3.302603
208	C	2.154518	–0.928307	4.542830
209	C	2.998459	–1.017538	5.666200
210	C	4.373142	–0.700979	5.577789
211	C	5.289403	–0.831942	6.779263
212	H	5.921250	–0.005465	4.230323
213	H	1.097300	–1.161428	4.632873
214	H	2.585622	–1.335172	6.621969
215	H	6.042899	–0.035953	6.800815
216	H	5.831464	–1.787668	6.756806
217	H	4.731243	–0.796301	7.721539
218	C	–2.998841	1.017369	5.666139
219	C	–2.154804	0.928147	4.542836
220	C	–2.676258	0.518089	3.302515
221	C	–4.038888	0.181789	3.193787
222	C	–4.871112	0.273166	4.325144
223	C	–4.373550	0.700997	5.577570
224	C	–5.289932	0.831911	6.778957
225	H	–2.586040	1.334843	6.621975
226	H	–1.097570	1.161137	4.633015
227	H	–4.439226	–0.168810	2.247665
228	H	–5.921632	0.005874	4.229865
229	H	–5.832869	1.787123	6.755882
230	H	–4.731746	0.797367	7.721255
231	H	–6.042708	0.035250	6.801013
232	H	4.439001	0.169243	2.247999
233	H	0.390653	–4.014024	5.649425
234	H	–0.725000	–5.236465	5.018308
235	H	–1.965802	–3.327530	5.804471

236	H	–1.029663	–2.183380	4.838262
237	H	1.965674	3.327655	5.804477
238	H	1.029421	2.183597	4.838291
239	H	–0.390650	4.014543	5.649390
240	H	0.725175	–5.236673	5.018001

Table S4. Optimised atomic coordinates of **2c-2tb** isomer of complex $[\mathbf{1}]^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	1.303823	1.206018	–2.185893
2	C	1.289522	3.173012	–2.620260
3	N	1.752486	3.779585	–3.768404
4	C	1.489006	5.167606	–3.725149
5	H	1.754333	5.831318	–4.531939
6	C	0.887448	5.430025	–2.529128
7	H	0.534243	6.354154	–2.104508
8	N	0.787040	4.204354	–1.855536
9	C	2.459687	3.209640	–4.948357
10	C	3.290392	1.304775	–2.421322
11	N	3.842842	1.530331	–3.657375
12	C	5.245664	1.589266	–3.570502
13	H	5.881622	1.740014	–4.427572
14	C	5.565737	1.410165	–2.249741
15	H	6.511289	1.400656	–1.738495
16	N	4.352275	1.250559	–1.552672
17	O	–0.960430	4.659379	–0.343042
18	C	0.356070	4.066609	–0.466363
19	H	0.327138	2.994134	–0.236879
20	C	1.298993	4.809315	0.517968
21	H	1.218672	5.888378	0.348087
22	C	0.824888	4.468252	1.938639
23	H	0.843836	3.387112	2.120034
24	C	–0.606364	5.023448	2.085873
25	H	–0.585533	6.115289	2.014748
26	C	–1.543454	4.426321	1.008233
27	H	–1.621424	3.340190	1.151195
28	O	2.690553	4.404872	0.295068
29	C	3.557571	5.409602	–0.206205
30	O	3.157745	6.554249	–0.442855
31	C	4.947659	4.888691	–0.439607
32	H	4.950832	4.235281	–1.321244
33	H	5.317337	4.293759	0.397955
34	H	5.616544	5.730866	–0.629111
35	O	1.693052	5.128642	2.911901
36	C	2.242569	4.353263	3.943222
37	O	2.076109	3.126524	4.005382
38	C	3.019732	5.200298	4.914111
39	H	2.497600	5.208899	5.878934
40	H	3.111909	6.226460	4.554275
41	H	4.006019	4.752046	5.076300
42	O	–1.148646	4.630984	3.390801
43	C	–1.396527	5.648259	4.336650
44	O	–1.110216	6.830410	4.119426
45	C	–2.073346	5.090995	5.557441
46	H	–1.746113	4.068176	5.760572
47	H	–3.155297	5.085000	5.370839
48	H	–1.878241	5.736658	6.416766
49	C	–2.946160	5.018026	1.015855
50	H	–3.451758	4.791206	0.076808

51	H	–3.518896	4.604980	1.851567
52	O	–2.900774	6.485781	1.151306
53	C	–3.592452	7.061800	2.221964
54	O	–4.218957	6.376991	3.047360
55	C	–3.426456	8.556061	2.241076
56	H	–4.280913	9.017819	2.741448
57	H	–3.310555	8.952906	1.229733
58	H	–2.521357	8.792180	2.815844
59	O	5.520718	1.701686	0.401722
60	C	4.227760	1.260910	–0.071668
61	H	3.457148	1.997717	0.186958
62	C	3.814678	–0.095684	0.551658
63	H	3.245141	–0.721339	–0.140125
64	C	5.022096	–0.870401	1.114030
65	H	4.677087	–1.795335	1.585563
66	C	5.866332	–0.051551	2.104937
67	H	6.907176	–0.385605	2.028725
68	C	5.761626	1.476826	1.845483
69	H	4.925168	1.882103	2.426880
70	O	2.956155	0.309817	1.680292
71	C	1.995755	–0.573061	2.167439
72	O	1.841777	–1.699386	1.666737
73	C	1.203216	0.040426	3.282659
74	H	0.375820	0.614573	2.844356
75	H	1.809558	0.740691	3.860189
76	H	0.782622	–0.750281	3.908685
77	O	5.932310	–1.202238	–0.009439
78	C	5.746420	–2.409075	–0.678267
79	O	4.779525	–3.148911	–0.442592
80	C	6.858952	–2.665420	–1.659859
81	H	7.756385	–2.984578	–1.114927
82	H	7.112877	–1.752844	–2.206963
83	H	6.569293	–3.457753	–2.352654
84	O	5.361609	–0.351707	3.455464
85	C	6.300443	–0.421809	4.502754
86	O	7.510244	–0.261499	4.300767
87	C	5.619829	–0.677593	5.818262
88	H	4.825681	–1.421539	5.706659
89	H	5.159970	0.254301	6.171142
90	H	6.354907	–1.008389	6.554491
91	C	7.075554	2.181160	2.175224
92	H	7.421094	1.877044	3.166652
93	H	7.832855	1.936987	1.425851
94	O	6.972513	3.652085	2.120945
95	C	6.511450	4.306749	3.259546
96	O	6.021610	3.689824	4.220446
97	C	6.713220	5.796317	3.155263
98	H	6.492509	6.154239	2.145691
99	H	7.765456	6.029355	3.362717
100	H	6.092391	6.313909	3.889060
101	Pt	–1.302242	–1.484515	–2.078828
102	C	–1.300876	–3.497053	–2.281804
103	N	–1.847701	–4.235036	–3.313877
104	C	–1.613284	–5.612255	–3.111285
105	H	–1.954007	–6.363381	–3.805030
106	C	–0.931677	–5.738245	–1.939633
107	H	–0.553647	–6.609566	–1.434858
108	N	–0.755814	–4.442292	–1.434436
109	C	–2.576497	–3.820977	–4.543297
110	C	–2.937495	–2.335693	–4.687276

111	C	–3.286418	–1.533484	–2.361279
112	N	–3.794198	–1.844524	–3.597669
113	C	–5.198034	–1.768005	–3.596098
114	H	–5.798148	–1.964472	–4.469467
115	C	–5.568365	–1.413620	–2.328615
116	H	–6.538740	–1.262667	–1.894739
117	N	–4.385922	–1.285194	–1.572031
118	O	1.211755	–4.919676	–0.307424
119	C	–0.043781	–4.194052	–0.177280
120	H	0.120154	–3.116842	–0.072690
121	C	–0.771811	–4.768302	1.062838
122	H	–0.858354	–5.854322	0.945562
123	C	0.090493	–4.439195	2.296003
124	H	0.261252	–3.362666	2.388978
125	C	1.417134	–5.199741	2.149449
126	H	1.225036	–6.277099	2.152759
127	C	2.139261	–4.777971	0.848615
128	H	2.439885	–3.727941	0.914972
129	O	–2.114492	–4.211943	1.245536
130	C	–3.193929	–5.103598	1.038454
131	O	–3.037900	–6.185512	0.460335
132	C	–4.478179	–4.559490	1.596061
133	H	–4.907919	–3.799852	0.933167
134	H	–4.303221	–4.085898	2.566451
135	H	–5.202554	–5.370371	1.694787
136	O	–0.587832	–4.936619	3.496640
137	C	–1.117673	–4.025479	4.400484
138	O	–1.081979	–2.795927	4.223546
139	C	–1.708403	–4.741905	5.587594
140	H	–0.918895	–5.281915	6.123010
141	H	–2.435450	–5.491052	5.255800
142	H	–2.182649	–4.024932	6.260083
143	O	2.310026	–4.866327	3.264368
144	C	2.613746	–5.882557	4.190256
145	O	2.096899	–7.004208	4.133293
146	C	3.654003	–5.419104	5.172079
147	H	3.572746	–4.344955	5.356946
148	H	4.641649	–5.629000	4.740680
149	H	3.562204	–5.981202	6.104407
150	C	3.365990	–5.625793	0.532557
151	H	3.616134	–5.523233	–0.524135
152	H	4.213174	–5.305949	1.142561
153	O	3.104563	–7.056676	0.777328
154	C	3.930196	–7.721861	1.690580
155	O	4.850585	–7.144015	2.291147
156	C	3.518182	–9.158687	1.855973
157	H	4.377741	–9.757568	2.166238
158	H	3.085219	–9.553940	0.933951
159	H	2.760432	–9.207426	2.648912
160	O	–5.640340	–1.735210	0.322822
161	C	–4.375726	–1.159624	–0.087119
162	H	–3.538228	–1.768401	0.275487
163	C	–4.187611	0.273053	0.464329
164	H	–3.404602	0.812946	–0.076784
165	C	–5.503724	1.070192	0.532314
166	H	–5.316006	2.030870	1.020456
167	C	–6.634637	0.327546	1.271760
168	H	–7.558135	0.440734	0.692645
169	C	–6.324172	–1.168365	1.518778
170	H	–5.665431	–1.250220	2.386537

171	O	–3.790785	0.070943	1.872813
172	C	–2.591129	0.581225	2.371704
173	O	–1.788701	1.192985	1.648458
174	C	–2.445695	0.262966	3.833181
175	H	–2.020882	–0.743032	3.955431
176	H	–3.421609	0.281604	4.325430
177	H	–1.771942	0.985540	4.299627
178	O	–5.992940	1.309683	–0.845331
179	C	–5.647547	2.514507	–1.463341
180	O	–4.845985	3.304018	–0.946590
181	C	–6.385353	2.689519	–2.762783
182	H	–7.430044	2.952584	–2.553926
183	H	–6.386006	1.756642	–3.334568
184	H	–5.926448	3.490484	–3.344253
185	O	–6.804044	0.971907	2.581227
186	C	–8.122293	1.167301	3.049686
187	O	–9.101574	0.892506	2.345276
188	C	–8.119863	1.693431	4.453742
189	H	–7.310260	2.412675	4.604890
190	H	–7.959704	0.842876	5.128417
191	H	–9.085313	2.150098	4.680855
192	C	–7.589997	–2.013168	1.708412
193	H	–8.419918	–1.396144	2.060729
194	H	–7.858727	–2.503650	0.770210
195	O	–7.378249	–3.123489	2.658876
196	C	–7.509329	–2.813899	4.012757
197	O	–7.672734	–1.647128	4.403440
198	C	–7.454500	–4.050268	4.870522
199	H	–6.729553	–4.768550	4.477392
200	H	–8.438454	–4.536511	4.862429
201	H	–7.211632	–3.779253	5.900217
202	S	1.186133	–1.278665	–1.843602
203	S	–1.180959	1.028973	–1.903532
204	C	3.301318	–3.748456	–4.392841
205	C	2.786836	–3.110345	–3.249160
206	C	1.862570	–2.058524	–3.394677
207	C	1.458383	–1.656821	–4.680833
208	C	1.982441	–2.301976	–5.817528
209	C	2.913179	–3.358612	–5.695371
210	C	3.478253	–4.058666	–6.916783
211	H	4.006322	–4.568060	–4.268352
212	H	0.733857	–0.854894	–4.795510
213	H	1.662275	–1.984883	–6.808373
214	H	3.288238	–5.139102	–6.879760
215	H	4.566546	–3.927785	–6.983066
216	H	3.040335	–3.673764	–7.844034
217	C	–2.181161	1.901464	–5.873333
218	C	–1.698420	1.233292	–4.732366
219	C	–1.837861	1.816600	–3.460412
220	C	–2.453999	3.076825	–3.336230
221	C	–2.927623	3.738418	–4.484839
222	C	–2.808167	3.164554	–5.771212
223	C	–3.348984	3.875346	–6.997449
224	H	–2.066443	1.440174	–6.852642
225	H	–1.200617	0.273799	–4.835968
226	H	–2.552662	3.544631	–2.361582
227	H	–3.390074	4.717237	–4.374479
228	H	–4.432071	3.718599	–7.099389
229	H	–2.879523	3.510491	–7.917886
230	H	–3.185505	4.957885	–6.939766

231	H	3.092905	–3.434556	–2.259533
232	H	–2.037025	–1.721452	–4.720654
233	H	–3.469237	–2.215960	–5.637019
234	H	–3.492673	–4.422487	–4.582881
235	H	–1.956873	–4.096512	–5.406406
236	C	2.997411	1.768075	–4.839099
237	H	2.178626	1.048069	–4.811539
238	H	3.585107	1.573527	–5.742662
239	H	3.291436	3.891185	–5.162214
240	H	1.774834	3.238407	–5.805659

Table S5. Optimised atomic coordinates of **2tb-2c** isomer of complex $[\mathbf{1}]^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	–1.612449	–1.082948	–1.885829
2	C	–2.171262	–3.003713	–2.276569
3	N	–2.708895	–3.426159	–3.486667
4	C	–3.135593	–4.764731	–3.407021
5	H	–3.582763	–5.282385	–4.239711
6	C	–2.876151	–5.193961	–2.142951
7	H	–3.086367	–6.135758	–1.656846
8	N	–2.276532	–4.115565	–1.461725
9	C	–2.852722	–2.705013	–4.771961
10	C	–3.091013	–1.182765	–4.689847
11	C	–3.519136	–0.608081	–2.312578
12	N	–3.980834	–0.779769	–3.594900
13	C	–5.347230	–0.472107	–3.685358
14	H	–5.903883	–0.525894	–4.606419
15	C	–5.746813	–0.093377	–2.435990
16	H	–6.712185	0.251938	–2.105960
17	N	–4.611855	–0.165078	–1.597108
18	O	–4.726927	–1.159921	0.527869
19	C	–4.600364	0.122926	–0.156885
20	H	–3.643750	0.595649	0.099416
21	C	–5.787329	1.007726	0.283473
22	H	–6.733390	0.568378	–0.049464
23	C	–5.847972	1.160933	1.814595
24	H	–5.040653	1.805592	2.171974
25	C	–5.783459	–0.204525	2.525251
26	H	–6.724648	–0.748404	2.394194
27	C	–4.592342	–1.024649	1.991332
28	H	–3.653439	–0.505857	2.230957
29	O	–5.644638	2.357841	–0.284025
30	C	–6.714317	2.885015	–1.023055
31	O	–7.651998	2.183620	–1.423745
32	C	–6.543930	4.364552	–1.238285
33	H	–5.500317	4.604363	–1.462265
34	H	–6.814721	4.895546	–0.316958
35	H	–7.200740	4.700763	–2.043010
36	O	–7.158617	1.794496	2.046535
37	C	–7.309284	2.696224	3.098635
38	O	–6.354419	3.056275	3.804533
39	C	–8.747584	3.107049	3.248059
40	H	–9.288129	2.291949	3.746522
41	H	–9.215279	3.262255	2.271511
42	H	–8.819152	4.009302	3.858734
43	O	–5.514450	–0.027615	3.964370
44	C	–6.600808	0.013368	4.853548
45	O	–7.770859	–0.106182	4.472139

46	C	–6.131039	0.253660	6.263098
47	H	–5.891519	1.318583	6.377426
48	H	–5.226286	–0.320735	6.481966
49	H	–6.925150	–0.006291	6.965957
50	C	–4.512400	–2.426093	2.566056
51	H	–3.730191	–2.992511	2.061484
52	H	–4.312445	–2.380619	3.638400
53	O	–5.816070	–3.099222	2.398035
54	C	–5.850688	–4.374395	1.872827
55	O	–4.819440	–4.986490	1.532727
56	C	–7.259908	–4.900029	1.794259
57	H	–7.271032	–5.857147	1.270157
58	H	–7.905180	–4.179605	1.280987
59	H	–7.663518	–5.031815	2.805364
60	O	–1.502571	–3.051343	0.515881
61	C	–2.033850	–4.281764	0.000122
62	H	–3.012406	–4.478805	0.456537
63	C	–1.124975	–5.519485	0.289152
64	H	–1.185660	–6.225874	–0.540144
65	C	0.364607	–5.235708	0.543951
66	H	0.764056	–6.031852	1.182044
67	C	0.675735	–3.890692	1.238817
68	H	1.247275	–3.229055	0.582943
69	C	–0.624120	–3.196173	1.695258
70	H	–1.113375	–3.819079	2.456009
71	O	–1.641118	–6.174303	1.504758
72	C	–2.643565	–7.142316	1.300309
73	O	–3.035922	–7.417311	0.157584
74	C	–3.123327	–7.724717	2.595692
75	H	–3.911172	–7.072331	2.991493
76	H	–2.314234	–7.776822	3.328415
77	H	–3.548502	–8.715476	2.420758
78	O	0.962830	–5.368857	–0.805977
79	C	2.314090	–5.697296	–0.906913
80	O	3.093858	–5.587389	0.049966
81	C	2.633909	–6.229558	–2.279826
82	H	2.082941	–5.682332	–3.047773
83	H	2.328350	–7.283135	–2.328153
84	H	3.707916	–6.172117	–2.466415
85	O	1.450409	–4.208109	2.448197
86	C	2.544322	–3.420138	2.788111
87	O	2.871110	–2.425684	2.110702
88	C	3.184687	–3.900322	4.057203
89	H	3.154172	–4.991646	4.112445
90	H	2.603147	–3.503593	4.900665
91	H	4.213818	–3.543058	4.126520
92	C	–0.418955	–1.779781	2.227886
93	H	0.590969	–1.632376	2.612423
94	H	–0.638841	–1.066150	1.432634
95	O	–1.392908	–1.479225	3.301272
96	C	–0.933364	–1.539908	4.618305
97	O	0.234391	–1.866323	4.891251
98	C	–1.991264	–1.130919	5.607486
99	H	–2.967783	–1.025677	5.131718
100	H	–1.698399	–0.162118	6.030094
101	H	–2.032859	–1.857274	6.425669
102	Pt	1.520510	0.980477	–1.846038
103	C	2.019478	2.904809	–2.260937
104	N	2.498763	3.323133	–3.494502
105	C	2.854900	4.683845	–3.457584

106	H	3.249416	5.204561	–4.314588
107	C	2.611853	5.129723	–2.196075
108	H	2.792700	6.091509	–1.737368
109	N	2.090646	4.037092	–1.471247
110	C	2.646490	2.576940	–4.764906
111	C	2.974686	1.071454	–4.657967
112	C	3.439368	0.560374	–2.273956
113	N	3.888223	0.729395	–3.560741
114	C	5.260081	0.448616	–3.657256
115	H	5.808362	0.500471	–4.583390
116	C	5.676751	0.093935	–2.406195
117	H	6.646997	–0.241627	–2.080999
118	N	4.547162	0.155373	–1.559330
119	O	4.726695	1.202798	0.535283
120	C	4.557529	–0.095224	–0.112351
121	H	3.595636	–0.540100	0.173087
122	C	5.728060	–1.001091	0.326195
123	H	6.678520	–0.607800	–0.049252
124	C	5.830677	–1.107461	1.859457
125	H	5.022517	–1.730645	2.254553
126	C	5.815789	0.277975	2.531844
127	H	6.766068	0.795835	2.365182
128	C	4.630326	1.109491	2.003959
129	H	3.686642	0.619903	2.283679
130	O	5.520395	–2.363555	–0.181881
131	C	6.546495	–2.965692	–0.927002
132	O	7.468224	–2.306373	–1.427940
133	C	6.355654	–4.456298	–1.005882
134	H	5.335808	–4.746555	–0.744125
135	H	7.032938	–4.929735	–0.282450
136	H	6.639708	–4.818146	–1.998701
137	O	7.137476	–1.758222	2.067977
138	C	7.309265	–2.638402	3.134630
139	O	6.375501	–2.963012	3.884049
140	C	8.744325	–3.074215	3.241050
141	H	9.317421	–2.261564	3.705970
142	H	9.173905	–3.256106	2.251748
143	H	8.819656	–3.967031	3.864997
144	O	5.575418	0.144430	3.981234
145	C	6.681968	0.082757	4.845159
146	O	7.844492	0.173905	4.434765
147	C	6.240246	–0.139962	6.266314
148	H	5.952472	–1.192578	6.382660
149	H	5.370867	0.477006	6.511734
150	H	7.064491	0.080128	6.947606
151	C	4.593832	2.527312	2.545869
152	H	3.782811	3.087086	2.080209
153	H	4.468905	2.508197	3.630551
154	O	5.881869	3.195711	2.278491
155	C	5.887363	4.392723	1.588862
156	O	4.841844	4.946442	1.198678
157	C	7.288738	4.913230	1.406116
158	H	7.271175	5.826279	0.808814
159	H	7.911165	4.155622	0.917957
160	H	7.739855	5.120325	2.383550
161	O	1.456059	2.952221	0.541734
162	C	1.931220	4.198406	0.004359
163	H	2.933463	4.407019	0.399650
164	C	1.029498	5.426835	0.358088
165	H	0.965058	6.101682	–0.497056

166	C	–0.401823	5.147792	0.876575
167	H	–0.579707	5.889284	1.661585
168	C	–0.649003	3.748242	1.448869
169	H	–1.220775	3.132867	0.748908
170	C	0.681360	3.053567	1.794496
171	H	1.229692	3.651531	2.535693
172	O	1.695383	6.143841	1.464717
173	C	2.606397	7.149897	1.105887
174	O	2.858463	7.387601	–0.083522
175	C	3.184464	7.826115	2.313420
176	H	3.921012	7.156908	2.773839
177	H	2.403789	8.035231	3.050438
178	H	3.681287	8.750661	2.013845
179	O	–1.396711	5.358440	–0.197792
180	C	–1.731398	6.696714	–0.464779
181	O	–1.159810	7.633389	0.106927
182	C	–2.835642	6.797611	–1.482524
183	H	–3.789781	6.532230	–1.009356
184	H	–2.659821	6.103414	–2.309359
185	H	–2.900414	7.823425	–1.850524
186	O	–1.413611	3.943778	2.695409
187	C	–2.481032	3.105314	2.989527
188	O	–2.833154	2.195006	2.211833
189	C	–3.078957	3.427565	4.327739
190	H	–2.922821	4.479552	4.578070
191	H	–2.559297	2.820306	5.081190
192	H	–4.143994	3.185659	4.335719
193	C	0.520369	1.615799	2.288405
194	H	–0.478546	1.426170	2.682613
195	H	0.744807	0.936379	1.464687
196	O	1.515653	1.304013	3.336359
197	C	1.068724	1.259080	4.658971
198	O	–0.106895	1.525815	4.961888
199	C	2.150408	0.814027	5.604535
200	H	3.132232	0.824634	5.128034
201	H	1.922255	–0.214353	5.912682
202	H	2.141573	1.443981	6.499622
203	S	0.868128	–1.431196	–1.520809
204	S	–0.950278	1.309760	–1.483320
205	C	3.551033	–3.252686	–4.086382
206	C	2.925113	–2.717787	–2.945700
207	C	1.620167	–2.195091	–3.040461
208	C	0.950716	–2.231448	–4.276384
209	C	1.581167	–2.781742	–5.408790
210	C	2.892901	–3.302511	–5.336829
211	C	3.563414	–3.918462	–6.550287
212	H	4.563902	–3.641543	–4.001669
213	H	–0.049077	–1.815393	–4.351059
214	H	1.051376	–2.804958	–6.359620
215	H	3.434231	–5.009943	–6.560755
216	H	4.642005	–3.722375	–6.559011
217	H	3.141600	–3.533824	–7.485781
218	C	–1.642984	2.674334	–5.367731
219	C	–1.079200	2.012101	–4.261018
220	C	–1.631781	2.181005	–2.978354
221	C	–2.751189	3.017324	–2.810540
222	C	–3.310310	3.670568	–3.925132
223	C	–2.767409	3.518154	–5.221315
224	C	–3.359948	4.254321	–6.407999
225	H	–1.208411	2.534354	–6.356140

226	H	–0.222047	1.356732	–4.389691
227	H	–3.177993	3.157352	–1.821222
228	H	–4.182822	4.307065	–3.787798
229	H	–4.455374	4.275938	–6.363501
230	H	–3.069808	3.791786	–7.357956
231	H	–3.017439	5.298214	–6.435361
232	H	3.449257	–2.706603	–1.993372
233	H	2.065516	0.485600	–4.514670
234	H	3.427645	0.758475	–5.604759
235	H	3.449446	3.082740	–5.310864
236	H	1.727554	2.683090	–5.355188
237	H	–3.699932	–3.175047	–5.281830
238	H	–1.961207	–2.878690	–5.388403
239	H	–2.150444	–0.646881	–4.555052
240	H	–3.527806	–0.858136	–5.640334

Table S6. Optimised atomic coordinates of **4tb** isomer of complex [**1**]$^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	–1.785132	0.440688	1.877148
2	C	–3.025325	1.980102	2.303734
3	N	–3.769271	2.179405	3.450929
4	C	–4.571191	3.333036	3.322183
5	H	–5.213304	3.680339	4.115028
6	C	–4.340473	3.850113	2.082450
7	H	–4.728618	4.721142	1.588934
8	N	–3.400579	3.012560	1.466928
9	C	–3.794056	1.433584	4.734953
10	C	–3.192233	0.018796	4.733770
11	C	–3.287582	–0.780202	2.389468
12	N	–3.744237	–0.842366	3.680824
13	C	–4.809119	–1.754358	3.790430
14	H	–5.303892	–1.969378	4.723552
15	C	–5.019293	–2.261100	2.538132
16	H	–5.733423	–2.987465	2.186442
17	N	–4.071991	–1.659912	1.684202
18	O	–5.215718	–0.871890	–0.181144
19	C	–4.099108	–1.722329	0.209396
20	H	–3.172903	–1.270042	–0.151373
21	C	–4.204793	–3.166096	–0.343880
22	H	–3.605444	–3.842009	0.272836
23	C	–5.631299	–3.730859	–0.554960
24	H	–5.555106	–4.442320	–1.381564
25	C	–6.701485	–2.679864	–0.893114
26	H	–7.374983	–2.534662	–0.040575
27	C	–6.073235	–1.328091	–1.299559
28	H	–5.473415	–1.448611	–2.208311
29	O	–3.647965	–3.148073	–1.711275
30	C	–2.322952	–3.545648	–1.895310
31	O	–1.598393	–3.857660	–0.939604
32	C	–1.946450	–3.532991	–3.351068
33	H	–1.674141	–2.508304	–3.634924
34	H	–2.794850	–3.834932	–3.970758
35	H	–1.100668	–4.204869	–3.515752
36	O	–6.103486	–4.462871	0.643357
37	C	–5.659524	–5.789149	0.791178
38	O	–4.782451	–6.259762	0.055313
39	C	–6.389406	–6.489826	1.904270
40	H	–7.426126	–6.677864	1.599032

41	H	–6.423041	–5.866028	2.803667
42	H	–5.904167	–7.442577	2.123612
43	O	–7.462625	–3.211235	–2.031690
44	C	–8.865860	–3.078352	–2.020323
45	O	–9.458162	–2.582459	–1.052383
46	C	–9.459309	–3.565415	–3.308911
47	H	–8.951304	–4.467584	–3.660897
48	H	–9.319479	–2.778568	–4.061358
49	H	–10.527517	–3.751219	–3.180095
50	C	–7.108592	–0.211956	–1.478578
51	H	–8.109295	–0.606857	–1.655136
52	H	–7.107202	0.419799	–0.587522
53	O	–6.743990	0.685363	–2.592756
54	C	–7.388153	0.463466	–3.819087
55	O	–8.160194	–0.490441	–3.986775
56	C	–7.019013	1.519127	–4.826704
57	H	–5.938155	1.502995	–5.012516
58	H	–7.275215	2.507007	–4.427817
59	H	–7.554003	1.336612	–5.760310
60	O	–2.989104	4.683319	–0.078270
61	C	–2.883913	3.252962	0.101417
62	H	–1.838188	2.929855	0.077663
63	C	–3.653370	2.481372	–1.011858
64	H	–4.031775	1.518218	–0.656610
65	C	–4.761011	3.312138	–1.679239
66	H	–5.155598	2.767675	–2.540028
67	C	–4.285374	4.709710	–2.150591
68	H	–5.062364	5.448778	–1.926834
69	C	–2.949310	5.132495	–1.488129
70	H	–2.112984	4.659725	–2.009567
71	O	–2.668432	2.280262	–2.098337
72	C	–2.277738	1.017456	–2.509052
73	O	–2.632464	–0.025150	–1.941111
74	C	–1.364986	1.128910	–3.704585
75	H	–0.383051	1.490936	–3.375773
76	H	–1.763329	1.856824	–4.416998
77	H	–1.252237	0.153312	–4.180723
78	O	–5.835393	3.441955	–0.672061
79	C	–7.119827	3.704056	–1.177480
80	O	–7.322971	3.846564	–2.388782
81	C	–8.139444	3.812639	–0.074517
82	H	–8.235116	4.863583	0.228515
83	H	–7.843605	3.225943	0.798395
84	H	–9.114347	3.485187	–0.444761
85	O	–4.116402	4.639333	–3.612572
86	C	–4.565036	5.734322	–4.371963
87	O	–5.014337	6.756472	–3.839708
88	C	–4.395262	5.474088	–5.843851
89	H	–4.907896	4.548582	–6.127413
90	H	–3.331358	5.353688	–6.079738
91	H	–4.802022	6.311668	–6.412889
92	C	–2.789535	6.650286	–1.461473
93	H	–2.931035	7.054722	–2.467243
94	H	–3.513689	7.102291	–0.779398
95	O	–1.486367	7.097080	–0.939107
96	C	–0.368129	6.937360	–1.737806
97	O	–0.407383	6.316104	–2.818647
98	C	0.850303	7.578201	–1.127437
99	H	1.504511	6.790093	–0.736911
100	H	0.571662	8.259565	–0.321733

101	H	1.404619	8.118104	–1.901792
102	Pt	1.807164	–0.095828	1.836467
103	C	2.974605	–1.662940	2.335541
104	N	3.689121	–1.837401	3.504508
105	C	4.435305	–3.033825	3.448861
106	H	5.050369	–3.368051	4.268288
107	C	4.194066	–3.605522	2.235606
108	H	4.550025	–4.517709	1.794786
109	N	3.304915	–2.757405	1.560496
110	C	3.706049	–1.040348	4.758921
111	C	3.186149	0.405960	4.678030
112	C	3.375936	1.068370	2.299954
113	N	3.813302	1.173470	3.595829
114	C	4.963039	1.979668	3.674204
115	H	5.459575	2.204246	4.604116
116	C	5.245730	2.379146	2.397703
117	H	6.042648	2.991347	2.007178
118	N	4.258349	1.818849	1.562318
119	O	5.393862	0.862962	–0.213756
120	C	4.328488	1.809420	0.092568
121	H	3.380754	1.418407	–0.285779
122	C	4.579523	3.220905	–0.507762
123	H	4.152716	3.984752	0.149134
124	C	6.045264	3.577376	–0.855082
125	H	5.997198	4.314278	–1.661400
126	C	6.931939	2.401279	–1.300524
127	H	7.733040	2.248781	–0.568616
128	C	6.131745	1.093264	–1.475809
129	H	5.430918	1.183215	–2.313528
130	O	3.878223	3.278710	–1.805726
131	C	2.672891	3.981543	–1.870648
132	O	2.150945	4.468348	–0.856229
133	C	2.154080	4.047795	–3.280056
134	H	1.944377	3.032832	–3.639467
135	H	2.921950	4.469531	–3.938102
136	H	1.254106	4.665602	–3.318876
137	O	6.709383	4.208363	0.310936
138	C	6.584291	5.608652	0.426333
139	O	5.826529	6.249535	–0.310690
140	C	7.481860	6.147939	1.506939
141	H	8.525311	6.096858	1.172233
142	H	7.402288	5.548264	2.419704
143	H	7.225938	7.188391	1.715189
144	O	7.518391	2.775042	–2.596099
145	C	8.884954	2.507526	–2.812188
146	O	9.596329	2.022348	–1.922137
147	C	9.282932	2.851506	–4.217038
148	H	8.782326	3.762083	–4.557335
149	H	8.970139	2.023574	–4.865887
150	H	10.367448	2.962534	–4.279541
151	C	7.035021	–0.134579	–1.645409
152	H	8.038255	0.143420	–1.970786
153	H	7.086922	–0.671861	–0.695612
154	O	6.473873	–1.106280	–2.608432
155	C	6.965883	–1.041969	–3.920385
156	O	7.734669	–0.142411	–4.284985
157	C	6.459692	–2.189168	–4.754143
158	H	5.364149	–2.226178	–4.735321
159	H	6.831725	–3.131095	–4.333710
160	H	6.808801	–2.075958	–5.782022

161	O	2.597269	–4.507409	0.228769
162	C	2.764331	–3.069527	0.220763
163	H	1.799299	–2.562886	0.125963
164	C	3.674034	–2.604726	–0.953909
165	H	4.225939	–1.696634	–0.695594
166	C	4.602785	–3.700830	–1.495684
167	H	5.061697	–3.347737	–2.419885
168	C	3.885407	–5.042621	–1.781964
169	H	4.520633	–5.866534	–1.436835
170	C	2.491833	–5.133155	–1.107877
171	H	1.752688	–4.603782	–1.716264
172	O	2.776983	–2.342518	–2.102880
173	C	2.514703	–1.050360	–2.528822
174	O	2.881576	–0.043502	–1.908136
175	C	1.734800	–1.082266	–3.819201
176	H	0.758817	–1.549946	–3.646837
177	H	2.260313	–1.695451	–4.558383
178	H	1.602679	–0.068669	–4.200774
179	O	5.664647	–3.897217	–0.486844
180	C	6.935714	–4.240835	–0.986542
181	O	7.144754	–4.369093	–2.197614
182	C	7.927440	–4.443268	0.128149
183	H	7.837369	–5.467205	0.513840
184	H	7.739334	–3.749999	0.952397
185	H	8.941560	–4.314126	–0.256469
186	O	3.725660	–5.152395	–3.242530
187	C	3.987963	–6.398735	–3.837307
188	O	4.317705	–7.385111	–3.166602
189	C	3.783681	–6.338196	–5.325750
190	H	4.290265	–5.465418	–5.749404
191	H	2.712171	–6.244030	–5.541515
192	H	4.162649	–7.252692	–5.785385
193	C	2.080218	–6.585252	–0.873415
194	H	2.296152	–7.182763	–1.762674
195	H	2.619119	–6.993197	–0.014540
196	O	0.658825	–6.751230	–0.518641
197	C	–0.267825	–6.710376	–1.554034
198	O	0.046992	–6.357993	–2.705464
199	C	–1.627855	–7.158143	–1.089510
200	H	–1.982314	–6.527477	–0.269546
201	H	–1.569749	–8.187196	–0.716618
202	H	–2.341408	–7.112488	–1.913851
203	S	0.250397	1.789399	1.279525
204	S	–0.236710	–1.423225	1.295427
205	C	–0.375445	–3.523739	4.901824
206	C	–0.308330	–2.472788	3.967527
207	C	–0.362167	–2.754942	2.590891
208	C	–0.476452	–4.086244	2.148397
209	C	–0.532477	–5.127374	3.092932
210	C	–0.486823	–4.869092	4.481707
211	C	–0.544487	–6.005737	5.485026
212	H	–0.335475	–3.298631	5.966121
213	H	–0.202177	–1.444931	4.306710
214	H	–0.514795	–4.309039	1.087961
215	H	–0.600653	–6.153203	2.737134
216	H	–1.460053	–6.599249	5.363519
217	H	–0.518775	–5.638575	6.516849
218	H	0.301283	–6.693462	5.353645
219	C	0.363214	3.824839	4.923447
220	C	0.175049	2.817307	3.958618

221	C	0.481736	3.072013	2.609694
222	C	0.977478	4.332339	2.226547
223	C	1.158713	5.330682	3.201895
224	C	0.852802	5.100851	4.562473
225	C	1.025327	6.199107	5.594613
226	H	0.123381	3.621220	5.965631
227	H	–0.206766	1.842178	4.251882
228	H	1.220037	4.530755	1.187183
229	H	1.535697	6.304390	2.895657
230	H	1.989244	6.710127	5.480489
231	H	0.968906	5.808614	6.616775
232	H	0.242960	6.963258	5.489378
233	H	2.106458	0.426354	4.518524
234	H	3.398566	0.890269	5.637061
235	H	4.747068	–1.031023	5.101990
236	H	3.109961	–1.571683	5.512594
237	H	–2.109690	0.058436	4.597987
238	H	–3.397280	–0.430327	5.711307
239	H	–4.845792	1.378266	5.038787
240	H	–3.259543	2.025720	5.489584

Table S7. Optimised atomic coordinates of **2c-2tb** isomer of complex $[\mathbf{2}]^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	1.865291	–2.000448	–0.106841
2	C	3.099322	–2.263650	–1.684887
3	N	3.531393	–3.449918	–2.221880
4	C	4.294093	–3.221625	–3.382495
5	H	4.721398	–4.020518	–3.964115
6	C	4.344947	–1.871425	–3.571084
7	H	4.819040	–1.289384	–4.342041
8	N	3.618338	–1.291338	–2.519303
9	C	3.183382	–4.810085	–1.735998
10	H	2.946133	–5.402483	–2.625639
11	H	2.261178	–4.707402	–1.165168
12	C	4.282346	–5.509763	–0.943674
13	C	5.279958	–6.204328	–1.663284
14	H	5.246656	–6.214722	–2.750924
15	C	6.304221	–6.906541	–1.008394
16	H	7.060447	–7.432179	–1.584212
17	C	6.326733	–6.946111	0.397787
18	H	7.099281	–7.504596	0.918440
19	C	5.328600	–6.276676	1.123596
20	H	5.333108	–6.342872	2.209862
21	C	4.310118	–5.542957	0.475675
22	C	3.267375	–4.842988	1.341325
23	H	2.322672	–4.703132	0.818367
24	H	3.066330	–5.442124	2.235308
25	C	3.315280	–2.292132	1.275329
26	N	3.695946	–3.500616	1.810501
27	C	4.617434	–3.315954	2.853585
28	H	5.039347	–4.136316	3.408674
29	C	4.829372	–1.972148	2.970030
30	H	5.471806	–1.401079	3.614109
31	N	4.035393	–1.352387	1.990637
32	O	2.607279	0.558262	–3.548640
33	C	3.379998	0.142959	–2.394011
34	H	2.807672	0.299751	–1.469261
35	C	4.696589	0.960826	–2.353831

36	H	5.264014	0.817873	–3.279388
37	C	4.343550	2.444592	–2.184759
38	H	3.865434	2.626794	–1.216767
39	C	3.421472	2.868295	–3.348282
40	H	3.977764	2.820793	–4.289961
41	C	2.166128	1.971564	–3.429254
42	H	1.563011	2.063618	–2.515598
43	O	5.496449	0.484291	–1.220127
44	C	6.668983	–0.248462	–1.522320
45	O	7.051087	–0.410205	–2.685888
46	C	7.302480	–0.817827	–0.282789
47	H	6.863455	–1.806469	–0.088454
48	H	7.128487	–0.194654	0.595776
49	H	8.371663	–0.958856	–0.457792
50	O	5.585059	3.220096	–2.265845
51	C	5.765017	4.300977	–1.395551
52	O	4.953006	4.559829	–0.491159
53	C	7.033646	5.046199	–1.696888
54	H	6.852854	6.122648	–1.616293
55	H	7.409491	4.798925	–2.690913
56	H	7.777012	4.773376	–0.938257
57	O	2.961053	4.242329	–3.121616
58	C	3.387779	5.245148	–4.016601
59	O	4.197337	5.014044	–4.921679
60	C	2.697318	6.548468	–3.729933
61	H	2.499021	6.664092	–2.661451
62	H	1.740675	6.548397	–4.268760
63	H	3.301706	7.378486	–4.102933
64	C	1.250290	2.290586	–4.600434
65	H	0.553925	1.469165	–4.770969
66	H	0.690860	3.205038	–4.389094
67	O	2.031957	2.470911	–5.839431
68	C	1.872335	3.665608	–6.543914
69	O	1.112344	4.568395	–6.155083
70	C	2.757196	3.706637	–7.759929
71	H	2.329866	4.379100	–8.507494
72	H	2.900791	2.706680	–8.176442
73	H	3.735492	4.102747	–7.457841
74	O	5.393318	0.491635	2.263020
75	C	4.120407	0.099769	1.696163
76	H	4.142317	0.219307	0.609487
77	C	2.950107	0.945895	2.257864
78	H	2.030022	0.367613	2.376229
79	C	3.327457	1.656300	3.575278
80	H	2.483195	2.257550	3.923318
81	C	4.582593	2.532718	3.444162
82	H	5.023361	2.655282	4.439992
83	C	5.628991	1.937516	2.450254
84	H	5.542220	2.451164	1.486126
85	O	2.762295	1.980680	1.215130
86	C	1.649178	2.820524	1.277820
87	O	0.706305	2.588624	2.051601
88	C	1.763896	3.962734	0.308133
89	H	1.344579	3.678954	–0.665670
90	H	2.807619	4.249200	0.165085
91	H	1.184480	4.807937	0.688578
92	O	3.652176	0.636536	4.599082
93	C	2.625555	0.186027	5.430818
94	O	1.443991	0.504940	5.245557
95	C	3.164228	–0.687707	6.532428

96	H	3.728021	–0.073172	7.244920
97	H	3.850963	–1.438035	6.128295
98	H	2.338897	–1.173476	7.055721
99	O	4.118114	3.844375	2.961824
100	C	4.904545	4.969233	3.278838
101	O	5.905058	4.871174	3.999779
102	C	4.371104	6.202200	2.608166
103	H	3.297343	6.308351	2.795101
104	H	4.522182	6.101778	1.525767
105	H	4.904041	7.080688	2.975975
106	C	7.034937	2.059075	3.043362
107	H	7.231251	3.106767	3.286539
108	H	7.113698	1.441524	3.942110
109	O	8.107751	1.544212	2.170974
110	C	8.607713	2.387998	1.189907
111	O	8.051314	3.459682	0.896591
112	C	9.880265	1.853391	0.583987
113	H	9.924929	2.100196	–0.480404
114	H	9.970196	0.776204	0.736691
115	H	10.733728	2.338835	1.075174
116	Pt	–1.865282	–2.000460	0.106992
117	C	–3.099316	–2.263433	1.685079
118	N	–3.531386	–3.449632	2.222233
119	C	–4.294083	–3.221184	3.382817
120	H	–4.721381	–4.020002	3.964545
121	C	–4.344933	–1.870959	3.571227
122	H	–4.818989	–1.288816	4.342131
123	N	–3.618325	–1.291012	2.519368
124	C	–3.183381	–4.809863	1.736530
125	H	–2.946134	–5.402142	2.626251
126	H	–2.261178	–4.707257	1.165685
127	C	–4.282337	–5.509665	0.944302
128	C	–5.279954	–6.204127	1.664006
129	H	–5.246681	–6.214333	2.751649
130	C	–6.304184	–6.906475	1.009210
131	H	–7.060417	–7.432026	1.585098
132	C	–6.326654	–6.946294	–0.396967
133	H	–7.099171	–7.504893	–0.917542
134	C	–5.328521	–6.276958	–1.122864
135	H	–5.332995	–6.343340	–2.209119
136	C	–4.310075	–5.543100	–0.475040
137	C	–3.267349	–4.843222	–1.340779
138	H	–2.322650	–4.703270	–0.817841
139	H	–3.066288	–5.442463	–2.234688
140	C	–3.315286	–2.292353	–1.275120
141	N	–3.695957	–3.500916	–1.810116
142	C	–4.617526	–3.316411	–2.853154
143	H	–5.039435	–4.136852	–3.408128
144	C	–4.829545	–1.972628	–2.969724
145	H	–5.472035	–1.401653	–3.613830
146	N	–4.035500	–1.352726	–1.990473
147	O	–2.607262	0.558692	3.548499
148	C	–3.379987	0.143275	2.393917
149	H	–2.807674	0.299976	1.469143
150	C	–4.696586	0.961126	2.353691
151	H	–5.263983	0.818232	3.279274
152	C	–4.343572	2.444884	2.184486
153	H	–3.865446	2.627005	1.216483
154	C	–3.421506	2.868690	3.347982
155	H	–3.977791	2.821227	4.289666

156	C	–2.166137	1.971999	3.428995
157	H	–1.563043	2.063990	2.515317
158	O	–5.496474	0.484464	1.220055
159	C	–6.669036	–0.248195	1.522361
160	O	–7.051122	–0.409781	2.685957
161	C	–7.302640	–0.817583	0.282898
162	H	–6.863479	–1.806138	0.088416
163	H	–7.128863	–0.194335	–0.595661
164	H	–8.371771	–0.958780	0.458058
165	O	–5.585074	3.220398	2.265500
166	C	–5.764998	4.301241	1.395144
167	O	–4.952969	4.560027	0.490751
168	C	–7.033668	5.046443	1.696356
169	H	–6.852865	6.122897	1.615836
170	H	–7.409641	4.799124	2.690321
171	H	–7.776937	4.773678	0.937608
172	O	–2.961150	4.242726	3.121218
173	C	–3.387862	5.245580	4.016177
174	O	–4.197394	5.014506	4.921285
175	C	–2.697438	6.548900	3.729419
176	H	–2.499202	6.664483	2.660921
177	H	–1.740763	6.548871	4.268190
178	H	–3.301819	7.378923	4.102419
179	C	–1.250292	2.291138	4.600131
180	H	–0.553846	1.469787	4.770677
181	H	–0.690940	3.205625	4.388734
182	O	–2.031944	2.471456	5.839136
183	C	–1.872303	3.666147	6.543630
184	O	–1.112308	4.568929	6.154795
185	C	–2.757110	3.707149	7.759684
186	H	–2.329737	4.379578	8.507255
187	H	–2.900707	2.707181	8.176167
188	H	–3.735410	4.103287	7.457647
189	O	–5.393377	0.491316	–2.263098
190	C	–4.120496	0.099470	–1.696182
191	H	–4.142424	0.219130	–0.609520
192	C	–2.950155	0.945490	–2.257953
193	H	–2.030069	0.367183	–2.376189
194	C	–3.327441	1.655699	–3.575489
195	H	–2.483152	2.256869	–3.923600
196	C	–4.582563	2.532169	–3.444552
197	H	–5.023309	2.654558	–4.440412
198	C	–5.628980	1.937179	–2.450548
199	H	–5.542174	2.450972	–1.486499
200	O	–2.762399	1.980416	–1.215358
201	C	–1.649276	2.820240	–1.278070
202	O	–0.706357	2.588263	–2.051775
203	C	–1.764014	3.962497	–0.308441
204	H	–1.344745	3.678758	0.665394
205	H	–2.807747	4.248962	–0.165445
206	H	–1.184579	4.807677	–0.688906
207	O	–3.652160	0.635776	–4.599134
208	C	–2.625542	0.185136	–5.430797
209	O	–1.443977	0.504075	–5.245585
210	C	–3.164221	–0.688762	–6.532277
211	H	–3.728006	–0.074329	–7.244863
212	H	–3.850963	–1.439021	–6.128029
213	H	–2.338892	–1.174616	–7.055494
214	O	–4.118067	3.843916	–2.962462
215	C	–4.904551	4.968693	–3.279632

216	O	–5.905098	4.870470	–4.000504
217	C	–4.371074	6.201814	–2.609270
218	H	–3.297360	6.308025	–2.796447
219	H	–4.521930	6.101566	–1.526826
220	H	–4.904153	7.080196	–2.977129
221	C	–7.034930	2.058738	–3.043653
222	H	–7.231197	3.106415	–3.286923
223	H	–7.113741	1.441090	–3.942328
224	O	–8.107737	1.544016	–2.171166
225	C	–8.607651	2.387939	–1.190200
226	O	–8.051212	3.459648	–0.897032
227	C	–9.880273	1.853521	–0.584265
228	H	–9.925015	2.100569	0.480064
229	H	–9.970234	0.776303	–0.736730
230	H	–10.733677	2.338883	–1.075638
231	S	0.084819	–1.528012	1.614269
232	S	–0.084804	–1.528270	–1.614191
233	C	–0.202765	–3.208522	5.371515
234	C	–0.137186	–2.299388	4.299796
235	C	0.045745	–2.780449	2.988673
236	C	0.155792	–4.163021	2.761074
237	C	0.093476	–5.062869	3.842311
238	C	–0.083762	–4.602747	5.167200
239	C	–0.137964	–5.568032	6.336352
240	H	–0.356165	–2.824466	6.377946
241	H	0.276045	–4.537695	1.748322
242	H	0.179326	–6.131755	3.654842
243	H	–0.985482	–5.349310	6.997694
244	H	0.771260	–5.498979	6.949236
245	H	–0.230556	–6.607000	6.001573
246	C	–0.093285	–5.063573	–3.841531
247	C	–0.155641	–4.163515	–2.760471
248	C	–0.045702	–2.780980	–2.988343
249	C	0.137178	–2.300168	–4.299566
250	C	0.202794	–3.209508	–5.371108
251	C	0.083891	–4.603702	–5.166515
252	C	0.138146	–5.569214	–6.335477
253	H	–0.179051	–6.132428	–3.653847
254	H	–0.275838	–4.537998	–1.747642
255	H	0.235537	–1.235577	–4.484635
256	H	0.356152	–2.825641	–6.377618
257	H	–0.771064	–5.500303	–6.948397
258	H	0.230756	–6.608114	–6.000492
259	H	0.985675	–5.350600	–6.996840
260	H	–0.235613	–1.234766	4.484656

Table S8. Optimised atomic coordinates of **4c** isomer of complex $[\mathbf{2}]^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	–1.870460	0.221006	–1.966964
2	C	–3.375464	–1.124150	–2.247170
3	N	–3.903210	–1.499289	–3.458126
4	C	–4.915622	–2.459083	–3.292858
5	H	–5.468700	–2.868368	–4.120528
6	C	–5.019635	–2.706873	–1.959053
7	H	–5.691512	–3.358448	–1.428141
8	N	–4.075753	–1.882507	–1.318067
9	C	–3.433350	–1.094553	–4.809107
10	H	–3.228525	–2.019839	–5.357526

11	H	–2.478115	–0.588861	–4.668700
12	C	–4.443313	–0.253682	–5.574413
13	C	–5.373800	–0.900959	–6.414501
14	H	–5.339519	–1.983565	–6.521964
15	C	–6.332216	–0.171475	–7.138914
16	H	–7.040330	–0.687862	–7.780583
17	C	–6.354732	1.231793	–7.043785
18	H	–7.080836	1.807363	–7.610588
19	C	–5.413790	1.886874	–6.230903
20	H	–5.407798	2.974837	–6.198645
21	C	–4.461850	1.161465	–5.484026
22	C	–3.430591	1.920834	–4.667514
23	H	–2.482753	1.389658	–4.616551
24	H	–3.231543	2.887688	–5.143283
25	C	–3.169216	1.781520	–2.128399
26	N	–3.813270	2.221190	–3.261957
27	C	–4.767157	3.205795	–2.950186
28	H	–5.382722	3.676614	–3.697448
29	C	–4.703267	3.413744	–1.605715
30	H	–5.243068	4.107863	–0.986489
31	N	–3.706654	2.555441	–1.108263
32	O	–2.840587	–3.205704	0.141150
33	C	–3.720043	–2.038178	0.088221
34	H	–3.184699	–1.134405	0.409209
35	C	–4.929594	–2.333111	1.005828
36	H	–5.429054	–3.250959	0.678733
37	C	–4.432957	–2.536853	2.448997
38	H	–3.952071	–1.634877	2.847229
39	C	–3.448510	–3.713684	2.493573
40	H	–3.963371	–4.656920	2.287985
41	C	–2.297993	–3.504239	1.479356
42	H	–1.676105	–2.656418	1.810947
43	O	–5.880689	–1.228149	0.974102
44	C	–7.180525	–1.496760	0.482412
45	O	–7.463324	–2.585035	–0.031694
46	C	–8.085485	–0.317350	0.680233
47	H	–7.585792	0.603527	0.360850
48	H	–8.316651	–0.213366	1.747656
49	H	–9.010312	–0.465716	0.119870
50	O	–5.609981	–2.850592	3.257674
51	C	–5.784109	–2.177569	4.480743
52	O	–4.938908	–1.382216	4.913193
53	C	–7.105016	–2.520746	5.107445
54	H	–7.482842	–3.478295	4.743939
55	H	–7.817560	–1.727839	4.842756
56	H	–7.006754	–2.533671	6.196322
57	O	–2.860372	–3.745069	3.835179
58	C	–2.797770	–4.973625	4.519782
59	O	–3.215401	–6.025113	4.018915
60	C	–2.138213	–4.798615	5.857725
61	H	–2.431008	–3.849024	6.313608
62	H	–1.052377	–4.792870	5.698064
63	H	–2.397403	–5.635585	6.509724
64	C	–1.407185	–4.727652	1.334739
65	H	–0.695903	–4.593093	0.514607
66	H	–0.851945	–4.907799	2.259369
67	O	–2.286784	–5.878915	1.055022
68	C	–1.799150	–7.143221	1.343787
69	O	–0.595637	–7.336692	1.597533
70	C	–2.890976	–8.175896	1.331872

71	H	–2.462600	–9.177615	1.261837
72	H	–3.591154	–7.998102	0.510219
73	H	–3.448021	–8.085424	2.273350
74	O	–4.356744	1.984162	1.079784
75	C	–3.281198	2.567558	0.288321
76	H	–2.364627	1.966814	0.365085
77	C	–3.061553	4.002482	0.825799
78	H	–4.010986	4.547058	0.786801
79	C	–2.587892	3.954876	2.286256
80	H	–1.580832	3.529819	2.375165
81	C	–3.580612	3.161887	3.155530
82	H	–4.450022	3.788078	3.374516
83	C	–4.010965	1.824824	2.507746
84	H	–3.166346	1.119831	2.583946
85	O	–2.065932	4.720625	0.033878
86	C	–2.494782	5.917449	–0.594368
87	O	–3.690021	6.225105	–0.651898
88	C	–1.329498	6.694015	–1.130550
89	H	–0.665142	6.041710	–1.706374
90	H	–0.759207	7.101805	–0.286496
91	H	–1.691595	7.512812	–1.755289
92	O	–2.574198	5.358256	2.722145
93	C	–1.575145	5.806071	3.583794
94	O	–0.669909	5.049800	3.982278
95	C	–1.735615	7.263180	3.899478
96	H	–2.783914	7.562561	3.842074
97	H	–1.154278	7.834982	3.164844
98	H	–1.332794	7.472485	4.893552
99	O	–2.933565	2.748449	4.410190
100	C	–3.174010	3.493024	5.578970
101	O	–3.879102	4.507122	5.580196
102	C	–2.455677	2.874913	6.747701
103	H	–1.374607	2.903557	6.568372
104	H	–2.746373	1.824612	6.859362
105	H	–2.692642	3.426014	7.659401
106	C	–5.213436	1.199462	3.195040
107	H	–5.644803	0.427076	2.555663
108	H	–4.927347	0.759409	4.152977
109	O	–6.216118	2.258268	3.440965
110	C	–7.479907	1.851460	3.837100
111	O	–7.799256	0.649439	3.889757
112	C	–8.356253	3.026960	4.182446
113	H	–9.385552	2.692938	4.324420
114	H	–8.308337	3.787242	3.396063
115	H	–7.997085	3.493047	5.108179
116	Pt	1.870641	–0.220381	–1.966977
117	C	3.375431	1.125110	–2.246762
118	N	3.903111	1.500900	–3.457545
119	C	4.915280	2.460880	–3.291847
120	H	5.468243	2.870676	–4.119340
121	C	5.019227	2.708108	–1.957937
122	H	5.690929	3.359627	–1.426738
123	N	4.075550	1.883227	–1.317323
124	C	3.433556	1.096499	–4.808733
125	H	3.228709	2.021919	–5.356916
126	H	2.478361	0.590640	–4.668664
127	C	4.443810	0.256010	–5.574086
128	C	5.374458	0.903712	–6.413674
129	H	5.340066	1.986351	–6.520764
130	C	6.333181	0.174620	–7.138069

131	H	7.041411	0.691332	–7.779348
132	C	6.355856	–1.228681	–7.043439
133	H	7.082204	–1.803948	–7.610236
134	C	5.414755	–1.884178	–6.231083
135	H	5.408888	–2.972153	–6.199243
136	C	4.462499	–1.159164	–5.484221
137	C	3.431047	–1.918966	–4.668349
138	H	2.483223	–1.387772	–4.617371
139	H	3.232090	–2.885550	–5.144703
140	C	3.169318	–1.780846	–2.129172
141	N	3.813377	–2.220117	–3.262878
142	C	4.767032	–3.205070	–2.951471
143	H	5.382551	–3.675692	–3.698894
144	C	4.702972	–3.413632	–1.607104
145	H	5.242572	–4.108162	–0.988165
146	N	3.706491	–2.555359	–1.109351
147	O	2.840311	3.205569	0.142577
148	C	3.719890	2.038162	0.089058
149	H	3.184660	1.134176	0.409630
150	C	4.929461	2.332785	1.006742
151	H	5.428826	3.250822	0.680035
152	C	4.432901	2.535845	2.450043
153	H	3.952055	1.633675	2.847886
154	C	3.448450	3.712648	2.495160
155	H	3.963300	4.655958	2.289875
156	C	2.297855	3.503549	1.480948
157	H	1.676029	2.655578	1.812272
158	O	5.880642	1.227911	0.974472
159	C	7.180518	1.496897	0.483094
160	O	7.463255	2.585412	–0.030530
161	C	8.085549	0.317456	0.680420
162	H	7.585956	–0.603309	0.360555
163	H	8.316647	0.212966	1.747811
164	H	9.010413	0.466150	0.120203
165	O	5.609969	2.849228	3.258789
166	C	5.784264	2.175491	4.481443
167	O	4.939188	1.379760	4.913456
168	C	7.105114	2.518525	5.108347
169	H	7.483201	3.475934	4.744756
170	H	7.817531	1.725403	4.843966
171	H	7.006637	2.531679	6.197208
172	O	2.860367	3.743589	3.836798
173	C	2.797782	4.971968	4.521771
174	O	3.215591	6.023562	4.021287
175	C	2.137977	4.796617	5.859550
176	H	2.430386	3.846739	6.315078
177	H	1.052161	4.791323	5.699714
178	H	2.397348	5.633227	6.511939
179	C	1.406996	4.726990	1.336899
180	H	0.695632	4.592761	0.516782
181	H	0.851835	4.906762	2.261650
182	O	2.286572	5.878371	1.057603
183	C	1.798631	7.142600	1.346110
184	O	0.594972	7.335905	1.599302
185	C	2.890345	8.175411	1.334690
186	H	2.461845	9.177113	1.265206
187	H	3.590464	7.998135	0.512866
188	H	3.447519	8.084488	2.276046
189	O	4.356697	–1.984756	1.078789
190	C	3.281055	–2.567839	0.287236

191	H	2.364546	–1.967025	0.364198
192	C	3.061252	–4.002895	0.824285
193	H	4.010573	–4.547643	0.784982
194	C	2.587798	–3.955712	2.284815
195	H	1.580814	–3.530532	2.374013
196	C	3.580754	–3.163162	3.154223
197	H	4.450117	–3.789548	3.372850
198	C	4.011159	–1.825918	2.506861
199	H	3.166639	–1.120851	2.583472
200	O	2.065378	–4.720565	0.032251
201	C	2.493863	–5.917275	–0.596455
202	O	3.689015	–6.225234	–0.654184
203	C	1.328329	–6.693376	–1.132762
204	H	0.663742	–6.040626	–1.707807
205	H	0.758380	–7.101785	–0.288774
206	H	1.690127	–7.511733	–1.758250
207	O	2.573969	–5.359216	2.720255
208	C	1.574910	–5.807178	3.581840
209	O	0.669775	–5.050924	3.980578
210	C	1.735278	–7.264384	3.897129
211	H	2.783530	–7.563868	3.839431
212	H	1.153698	–7.835946	3.162504
213	H	1.332653	–7.473877	4.891245
214	O	2.933913	–2.750136	4.409120
215	C	3.174499	–3.495131	5.577609
216	O	3.879599	–4.509225	5.578384
217	C	2.456437	–2.877332	6.746673
218	H	1.375342	–2.905623	6.567452
219	H	2.747418	–1.827151	6.858734
220	H	2.693372	–3.428864	7.658122
221	C	5.213827	–1.200948	3.194152
222	H	5.645028	–0.428257	2.555032
223	H	4.928015	–0.761360	4.152387
224	O	6.216554	–2.259913	3.439220
225	C	7.480246	–1.853277	3.835879
226	O	7.799434	–0.651260	3.889520
227	C	8.356613	–3.028913	4.180690
228	H	9.386313	–2.695274	4.320693
229	H	8.306938	–3.789922	3.395146
230	H	7.998844	–3.493886	5.107538
231	S	–0.193748	–1.616856	–1.596230
232	S	0.193876	1.617264	–1.595152
233	C	–1.374696	–4.915547	–3.791974
234	C	–1.130668	–4.007869	–2.744245
235	C	–0.474122	–2.791406	–3.013145
236	C	–0.092844	–2.483815	–4.330775
237	C	–0.335684	–3.401858	–5.369876
238	C	–0.970791	–4.639721	–5.118914
239	C	–1.199393	–5.646339	–6.230320
240	H	–1.886809	–5.850009	–3.571773
241	H	0.368668	–1.525031	–4.547503
242	H	–0.032224	–3.153289	–6.385198
243	H	–2.155317	–6.169742	–6.110942
244	H	–0.411982	–6.412965	–6.232835
245	H	–1.193140	–5.170476	–7.217371
246	C	0.335791	3.403954	–5.368006
247	C	0.093211	2.485323	–4.329327
248	C	0.474123	2.792524	–3.011518
249	C	1.130043	4.009200	–2.741983
250	C	1.373774	4.917455	–3.789244

251	C	0.970248	4.641993	–5.116401
252	C	1.198803	5.649205	–6.227283
253	H	0.032580	3.155694	–6.383473
254	H	–0.367867	1.526436	–4.546542
255	H	1.474896	4.228974	–1.737033
256	H	1.885367	5.852092	–3.568546
257	H	0.415078	6.419583	–6.225251
258	H	1.186158	5.174858	–7.214983
259	H	2.157714	6.167926	–6.111209
260	H	–1.475805	–4.227939	–1.739446

Table S9. Optimised atomic coordinates of **2tb-2c** isomer of complex [**2**]$^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	2.036450	1.806327	0.346090
2	C	3.236279	2.084179	1.977089
3	N	3.762624	3.307151	2.353245
4	C	4.762780	3.155641	3.323242
5	H	5.314051	3.987875	3.726294
6	C	4.864861	1.822759	3.583318
7	H	5.526537	1.277717	4.239965
8	N	3.906723	1.175380	2.775035
9	C	3.304264	4.646605	1.903549
10	H	2.886805	5.156772	2.779302
11	H	2.491750	4.467735	1.199103
12	C	4.400948	5.499731	1.290521
13	C	5.071580	6.446346	2.091204
14	H	4.792283	6.560994	3.137149
15	C	6.082014	7.265109	1.555051
16	H	6.588395	7.990225	2.185672
17	C	6.419885	7.151097	0.194735
18	H	7.189906	7.786891	–0.232716
19	C	5.741271	6.222409	–0.615285
20	H	5.983239	6.162924	–1.674793
21	C	4.738388	5.387245	–0.082680
22	C	4.000561	4.430152	–1.002619
23	H	2.939101	4.372275	–0.770738
24	H	4.083132	4.779731	–2.037634
25	C	3.780045	1.896486	–0.707663
26	N	4.507954	3.034382	–0.980120
27	C	5.800012	2.715832	–1.428338
28	H	6.527030	3.466919	–1.685539
29	C	5.880305	1.358784	–1.474865
30	H	6.697021	0.724594	–1.768519
31	N	4.632441	0.858379	–1.060907
32	O	5.218317	–1.213343	–0.141023
33	C	4.330455	–0.575655	–1.107456
34	H	3.279070	–0.723121	–0.838635
35	C	4.652925	–1.146009	–2.515741
36	H	5.652413	–0.815615	–2.815270
37	C	4.629479	–2.682349	–2.587927
38	H	3.605128	–3.072379	–2.604276
39	C	5.459428	–3.292234	–1.445269
40	H	6.526647	–3.140179	–1.633506
41	C	5.052714	–2.681446	–0.089617
42	H	3.998391	–2.914120	0.113542
43	O	3.682217	–0.649315	–3.493605
44	C	4.146577	0.181623	–4.520067
45	O	5.270611	0.699346	–4.503278

46	C	3.115558	0.314438	–5.610152
47	H	2.128532	0.028091	–5.243273
48	H	3.394244	–0.356931	–6.432971
49	H	3.113789	1.337645	–5.995681
50	O	5.300942	–2.951685	–3.879721
51	C	4.986851	–4.086960	–4.618904
52	O	4.090882	–4.877167	–4.284991
53	C	5.896207	–4.214344	–5.811124
54	H	6.855652	–4.624196	–5.469719
55	H	6.094385	–3.237933	–6.261996
56	H	5.460023	–4.896883	–6.543458
57	O	5.189383	–4.735759	–1.316126
58	C	6.066996	–5.640219	–1.938861
59	O	7.064017	–5.263826	–2.565579
60	C	5.596017	–7.057132	–1.755076
61	H	4.734152	–7.227791	–2.412442
62	H	5.277443	–7.236492	–0.723740
63	H	6.394422	–7.749587	–2.028647
64	C	5.891530	–3.195486	1.066122
65	H	5.728239	–2.590759	1.962188
66	H	5.633921	–4.235586	1.289380
67	O	7.311804	–3.129670	0.682102
68	C	8.242503	–3.385842	1.681363
69	O	7.890957	–3.618633	2.849226
70	C	9.650811	–3.339803	1.152979
71	H	10.355344	–3.532148	1.963679
72	H	9.854904	–2.359401	0.708059
73	H	9.779680	–4.089152	0.363638
74	O	2.752677	–0.762214	2.002906
75	C	3.778589	–0.302030	2.894579
76	H	4.742522	–0.725711	2.586074
77	C	3.512166	–0.695360	4.384846
78	H	3.940937	0.060344	5.043064
79	C	2.031939	–0.849745	4.765921
80	H	1.962069	–1.458137	5.674138
81	C	1.144491	–1.519128	3.691751
82	H	0.333842	–0.857282	3.373334
83	C	1.997132	–1.947219	2.481217
84	H	2.697571	–2.726944	2.806177
85	O	4.172544	–1.981269	4.663761
86	C	5.512044	–1.889535	5.111002
87	O	6.082089	–0.787261	5.138300
88	C	6.077946	–3.223109	5.490655
89	H	6.742391	–3.569700	4.688356
90	H	5.285673	–3.956428	5.652133
91	H	6.685578	–3.113128	6.394275
92	O	1.634624	0.540558	5.089350
93	C	0.515907	0.734991	5.899425
94	O	–0.283579	–0.179389	6.144128
95	C	0.474492	2.145707	6.424712
96	H	0.679259	2.861140	5.623511
97	H	1.250963	2.265039	7.191164
98	H	–0.499784	2.348509	6.871336
99	O	0.603865	–2.738689	4.307389
100	C	–0.709275	–3.127556	4.030371
101	O	–1.432112	–2.478849	3.254815
102	C	–1.051632	–4.398962	4.749435
103	H	–0.767320	–4.329792	5.804279
104	H	–0.471241	–5.212957	4.297945
105	H	–2.117318	–4.611116	4.651567

106	C	1.191022	–2.441933	1.282739
107	H	0.188034	–2.752903	1.575267
108	H	1.143597	–1.655981	0.527612
109	O	1.880445	–3.572559	0.624238
110	C	1.482943	–4.862993	0.991578
111	O	0.628270	–5.049991	1.873204
112	C	2.170154	–5.918496	0.172797
113	H	3.098673	–5.549539	–0.267163
114	H	1.487858	–6.202608	–0.638749
115	H	2.348406	–6.804297	0.789424
116	Pt	–1.700896	1.732038	–0.433030
117	C	–2.827403	2.021880	–2.106121
118	N	–3.182084	3.270607	–2.580202
119	C	–4.138916	3.175440	–3.598877
120	H	–4.565554	4.039202	–4.079655
121	C	–4.382088	1.849804	–3.796820
122	H	–5.072704	1.347012	–4.457896
123	N	–3.548166	1.146452	–2.898848
124	C	–2.565892	4.568739	–2.199608
125	H	–2.121062	4.988011	–3.108264
126	H	–1.747143	4.332264	–1.522071
127	C	–3.539531	5.569146	–1.599431
128	C	–4.136760	6.533658	–2.437271
129	H	–3.892021	6.548207	–3.497915
130	C	–5.024972	7.495590	–1.924212
131	H	–5.475938	8.229929	–2.585589
132	C	–5.309928	7.512472	–0.547190
133	H	–5.982834	8.259914	–0.136624
134	C	–4.702933	6.567319	0.298784
135	H	–4.899413	6.607811	1.368713
136	C	–3.826721	5.586369	–0.210172
137	C	–3.179118	4.604463	0.751720
138	H	–2.158359	4.350964	0.464943
139	H	–3.133575	5.044853	1.753469
140	C	–3.397716	2.060866	0.640687
141	N	–3.907149	3.314736	0.888949
142	C	–5.172735	3.238689	1.489720
143	H	–5.745485	4.110855	1.754384
144	C	–5.458780	1.917591	1.649261
145	H	–6.320120	1.452331	2.093036
146	N	–4.358903	1.194021	1.147983
147	O	–5.193503	–0.800182	0.214334
148	C	–4.282210	–0.266323	1.229453
149	H	–3.250277	–0.573402	1.025363
150	C	–4.783569	–0.780665	2.604024
151	H	–5.805801	–0.423511	2.765780
152	C	–4.817363	–2.317837	2.670462
153	H	–3.809813	–2.748737	2.682067
154	C	–5.679619	–2.855748	1.516946
155	H	–6.730417	–2.612615	1.701054
156	C	–5.214495	–2.278717	0.163393
157	H	–4.199778	–2.641497	–0.049567
158	O	–3.938177	–0.299910	3.696907
159	C	–4.588274	0.314535	4.788306
160	O	–5.728276	0.784929	4.691543
161	C	–3.729213	0.282868	6.022413
162	H	–2.662585	0.268747	5.790547
163	H	–3.947197	–0.647098	6.564966
164	H	–3.985394	1.118362	6.679018
165	O	–5.501212	–2.583937	3.951786

166	C	–5.231519	–3.748793	4.664117
167	O	–4.360213	–4.560073	4.313711
168	C	–6.151463	–3.872370	5.848624
169	H	–7.129904	–4.218914	5.491437
170	H	–6.303390	–2.903202	6.332310
171	H	–5.752794	–4.600142	6.558315
172	O	–5.538468	–4.316529	1.381790
173	C	–6.510883	–5.143444	1.972488
174	O	–7.479223	–4.685035	2.588798
175	C	–6.175030	–6.596049	1.767418
176	H	–5.328664	–6.858431	2.414568
177	H	–5.882048	–6.789242	0.730826
178	H	–7.034071	–7.213563	2.036562
179	C	–6.132769	–2.680197	–0.978915
180	H	–5.925276	–2.089959	–1.874712
181	H	–6.001902	–3.740664	–1.216923
182	O	–7.525645	–2.454106	–0.557951
183	C	–8.507840	–2.613619	–1.527704
184	O	–8.218883	–2.900520	–2.700380
185	C	–9.885280	–2.396749	–0.961816
186	H	–10.632075	–2.539791	–1.744411
187	H	–9.968112	–1.383914	–0.551404
188	H	–10.068228	–3.097866	–0.139697
189	O	–2.635184	–0.832466	–1.951891
190	C	–3.603668	–0.339709	–2.890271
191	H	–4.608297	–0.613733	–2.546352
192	C	–3.411375	–0.907172	–4.335804
193	H	–3.667474	–0.141698	–5.068317
194	C	–2.017433	–1.472779	–4.695245
195	H	–2.204225	–2.295770	–5.391347
196	C	–1.182508	–2.001288	–3.522538
197	H	–0.333597	–1.344142	–3.308116
198	C	–2.060623	–2.162157	–2.267168
199	H	–2.864699	–2.880402	–2.477197
200	O	–4.347729	–2.034383	–4.514763
201	C	–5.605415	–1.709472	–5.072109
202	O	–5.925389	–0.521142	–5.229900
203	C	–6.420925	–2.925708	–5.385184
204	H	–7.125736	–3.105661	–4.563008
205	H	–5.783819	–3.802952	–5.513933
206	H	–7.004989	–2.742403	–6.291600
207	O	–1.212932	–0.444695	–5.397619
208	C	–1.500370	–0.283955	–6.766369
209	O	–2.412584	–0.913992	–7.313790
210	C	–0.591261	0.728356	–7.411153
211	H	0.456508	0.499207	–7.192504
212	H	–0.812558	1.727272	–7.016341
213	H	–0.754719	0.726080	–8.490284
214	O	–0.705699	–3.330848	–3.942869
215	C	0.578231	–3.755683	–3.586581
216	O	1.341944	–3.029090	–2.927746
217	C	0.839965	–5.150376	–4.071782
218	H	0.369678	–5.318798	–5.044506
219	H	0.383107	–5.843263	–3.353390
220	H	1.915219	–5.328881	–4.124259
221	C	–1.295410	–2.580711	–1.011487
222	H	–0.319055	–3.000967	–1.251618
223	H	–1.187935	–1.712711	–0.359130
224	O	–2.069768	–3.565040	–0.227695
225	C	–1.714606	–4.912424	–0.357663

226	O	–0.841449	–5.276050	–1.163329
227	C	–2.468200	–5.784276	0.604043
228	H	–3.438378	–5.353912	0.859461
229	H	–1.872114	–5.861336	1.522819
230	H	–2.577196	–6.787569	0.183417
231	S	–0.179015	1.443216	1.548094
232	S	0.501079	1.407801	–1.627958
233	C	–2.234520	3.488712	4.480622
234	C	–1.751765	2.492337	3.612708
235	C	–0.711018	2.790743	2.710810
236	C	–0.159749	4.082365	2.696773
237	C	–0.636301	5.067765	3.582998
238	C	–1.681744	4.790748	4.492403
239	C	–2.179312	5.843899	5.464281
240	H	–3.047520	3.249404	5.162763
241	H	0.614346	4.326589	1.979979
242	H	–0.199327	6.064333	3.559482
243	H	–1.656702	5.769090	6.428474
244	H	–3.250018	5.730390	5.670081
245	H	–2.011870	6.858217	5.084333
246	C	0.943389	5.245331	–3.220280
247	C	0.818591	4.179663	–2.309859
248	C	0.652213	2.863268	–2.774599
249	C	0.581950	2.625654	–4.160600
250	C	0.703455	3.697766	–5.064415
251	C	0.898266	5.024485	–4.615347
252	C	1.067682	6.165331	–5.600712
253	H	1.072166	6.258279	–2.843406
254	H	0.828853	4.371679	–1.240517
255	H	0.420717	1.615331	–4.524426
256	H	0.654871	3.503136	–6.134178
257	H	2.084765	6.178465	–6.016678
258	H	0.895599	7.138357	–5.127560
259	H	0.376606	6.073929	–6.447352
260	H	–2.184488	1.496343	3.627097

Table S10. Optimised atomic coordinates of **4tb** isomer of complex $[\mathbf{2}]^{2+}$ obtained from DFT calculations.

Number	atom	x	y	z
1	Pt	1.804064	−0.244724	1.791455
2	C	3.013697	−1.845831	2.032874
3	N	3.593338	−2.297362	3.193710
4	C	4.512414	−3.327747	2.919378
5	H	5.078230	−3.819875	3.692094
6	C	4.488469	−3.538967	1.572000
7	H	5.009309	−4.242697	0.950266
8	N	3.558980	−2.633058	1.033299
9	C	3.123468	−1.985836	4.570462
10	H	2.869276	−2.948124	5.029085
11	H	2.190222	−1.434612	4.452065
12	C	4.112273	−1.254270	5.464449
13	C	4.997286	−2.012828	6.259832
14	H	4.969027	−3.099566	6.206485
15	C	5.897066	−1.395183	7.145245
16	H	6.570462	−1.998040	7.747707
17	C	5.900503	0.006200	7.265498
18	H	6.575717	0.494548	7.962244
19	C	5.009297	0.769921	6.492486
20	H	4.993234	1.851346	6.615972

21	C	4.121546	0.159753	5.581158
22	C	3.191356	1.044157	4.763940
23	H	2.232829	0.566541	4.556876
24	H	2.988279	1.972323	5.308718
25	C	3.322375	1.027186	2.211462
26	N	3.761976	1.430743	3.448634
27	C	4.834616	2.329356	3.330228
28	H	5.328433	2.760143	4.184505
29	C	5.069110	2.500219	1.998188
30	H	5.782257	3.130100	1.495951
31	N	4.131497	1.704420	1.317091
32	O	5.239746	0.737383	−0.523229
33	C	4.091517	1.541951	−0.150091
34	H	3.179347	0.977317	−0.365621
35	C	4.003359	2.905014	−0.877906
36	H	3.364395	3.580646	−0.301302
37	C	5.350308	3.592292	−1.218114
38	H	5.208271	4.098265	−2.176826
39	C	6.563637	2.657668	−1.321675
40	H	7.162713	2.698953	−0.404523
41	C	6.153124	1.199830	−1.613630
42	H	5.629218	1.124175	−2.571745
43	O	3.353460	2.650979	−2.179546
44	C	2.095633	3.231475	−2.408104
45	O	1.473542	3.812824	−1.509909
46	C	1.644663	3.031340	−3.829991
47	H	0.999623	2.144689	−3.881894
48	H	2.499899	2.881957	−4.492148
49	H	1.053237	3.897027	−4.143814
50	O	5.703188	4.608212	−0.200403
51	C	5.126077	5.878876	−0.335068
52	O	4.243714	6.100184	−1.175089
53	C	5.726385	6.858081	0.636520
54	H	6.767730	7.059972	0.357923
55	H	5.734308	6.442231	1.649673
56	H	5.162344	7.792219	0.617002
57	O	7.359123	3.175582	−2.439345
58	C	8.758853	3.239947	−2.297401
59	O	9.314448	2.907991	−1.241209
60	C	9.401894	3.719757	−3.563945
61	H	8.840112	4.551688	−3.998898
62	H	9.388540	2.888901	−4.279695
63	H	10.434555	4.015182	−3.368409
64	C	7.338109	0.216313	−1.561362
65	H	8.296186	0.734738	−1.618050
66	H	7.281923	−0.360173	−0.635881
67	O	7.264103	−0.786557	−2.638674
68	C	7.829387	−0.423613	−3.866760
69	O	8.420896	0.656802	−4.011102
70	C	7.602187	−1.470878	−4.921150
71	H	6.563969	−1.395504	−5.270179
72	H	7.747051	−2.475367	−4.515092
73	H	8.274279	−1.292454	−5.763024
74	O	2.866682	−4.199760	−0.507833
75	C	3.026208	−2.763548	−0.338694
76	H	2.052776	−2.262063	−0.356651
77	C	3.887781	−2.146191	−1.472060
78	H	4.468048	−1.283345	−1.132299
79	C	4.786259	−3.169159	−2.185876
80	H	5.288185	−2.700865	−3.034337

81	C	4.018001	−4.413059	−2.680385
82	H	4.678171	−5.284690	−2.620885
83	C	2.698927	−4.664994	−1.900576
84	H	1.886224	−4.112880	−2.381330
85	O	2.848087	−1.713650	−2.447849
86	C	3.200477	−0.947301	−3.554526
87	O	4.321521	−0.442228	−3.691973
88	C	2.050646	−0.859806	−4.523651
89	H	1.118375	−0.641000	−3.992875
90	H	1.935045	−1.833626	−5.014799
91	H	2.254350	−0.095713	−5.276166
92	O	5.811431	−3.558869	−1.196541
93	C	7.048219	−3.982578	−1.716012
94	O	7.236775	−4.090638	−2.931544
95	C	8.027943	−4.298193	−0.616990
96	H	7.816425	−5.295039	−0.208515
97	H	7.950707	−3.571292	0.196480
98	H	9.040922	−4.303514	−1.024630
99	O	3.687343	−4.179959	−4.101362
100	C	3.798868	−5.273132	−4.981401
101	O	4.166635	−6.387313	−4.592416
102	C	3.386083	−4.892535	−6.376262
103	H	3.723474	−3.882580	−6.625398
104	H	2.290551	−4.920676	−6.440663
105	H	3.793564	−5.613780	−7.087633
106	C	2.393106	−6.162368	−1.825518
107	H	2.687604	−6.647863	−2.759820
108	H	2.935205	−6.606887	−0.987013
109	O	0.980198	−6.486685	−1.553637
110	C	0.089941	−6.373369	−2.613091
111	O	0.407655	−5.813312	−3.680826
112	C	−1.236034	−7.006693	−2.294543
113	H	−1.768585	−6.421950	−1.539126
114	H	−1.082517	−8.014802	−1.895705
115	H	−1.851620	−7.054645	−3.194990
116	Pt	−1.804037	0.244938	1.791314
117	C	−3.013580	1.846130	2.032495
118	N	−3.593137	2.297923	3.193273
119	C	−4.512101	3.328362	2.918800
120	H	−5.077847	3.820686	3.691442
121	C	−4.488140	3.539390	1.571393
122	H	−5.008898	4.243097	0.949566
123	N	−3.558799	2.633259	1.032806
124	C	−3.123334	1.986487	4.570066
125	H	−2.869076	2.948795	5.028611
126	H	−2.190132	1.435170	4.451751
127	C	−4.112257	1.255099	5.464070
128	C	−4.997281	2.013830	6.259284
129	H	−4.968914	3.100559	6.205813
130	C	−5.897201	1.396369	7.144678
131	H	−6.570601	1.999352	7.747009
132	C	−5.900778	−0.005003	7.265086
133	H	−6.576109	−0.493210	7.961817
134	C	−5.009562	−0.768889	6.492255
135	H	−4.993606	−1.850300	6.615868
136	C	−4.121662	−0.158905	5.580944
137	C	−3.191455	−1.043494	4.763940
138	H	−2.232902	−0.565946	4.556847
139	H	−2.988434	−1.971557	5.308914
140	C	−3.322376	−1.026914	2.211459

141	N	−3.761995	−1.430328	3.448678
142	C	−4.834590	−2.328998	3.330355
143	H	−5.328380	−2.759739	4.184671
144	C	−5.069028	−2.500063	1.998330
145	H	−5.782129	−3.130061	1.496178
146	N	−4.131435	−1.704305	1.317156
147	O	−5.239387	−0.737405	−0.523475
148	C	−4.091321	−1.542028	−0.150065
149	H	−3.179084	−0.977488	−0.365555
150	C	−4.003174	−2.905199	−0.877671
151	H	−3.364243	−3.580756	−0.300940
152	C	−5.350149	−3.592498	−1.217756
153	H	−5.208201	−4.098450	−2.176493
154	C	−6.563507	−2.657901	−1.321206
155	H	−7.162410	−2.699058	−0.403935
156	C	−6.153092	−1.200101	−1.613487
157	H	−5.629468	−1.124602	−2.571770
158	O	−3.353255	−2.651383	−2.179325
159	C	−2.095515	−3.232095	−2.407864
160	O	−1.473463	−3.813413	−1.509627
161	C	−1.644560	−3.032092	−3.829775
162	H	−1.000297	−2.144890	−3.881937
163	H	−2.499871	−2.883610	−4.492046
164	H	−1.052434	−3.897409	−4.143274
165	O	−5.702924	−4.608425	−0.200030
166	C	−5.125820	−5.879088	−0.334755
167	O	−4.243546	−6.100389	−1.174869
168	C	−5.726004	−6.858289	0.636911
169	H	−6.767344	−7.060282	0.358367
170	H	−5.733918	−6.442389	1.650042
171	H	−5.161893	−7.792387	0.617416
172	O	−7.359204	−3.176003	−2.438632
173	C	−8.758916	−3.240249	−2.296441
174	O	−9.314311	−2.908006	−1.240235
175	C	−9.402208	−3.720288	−3.562769
176	H	−8.840187	−4.551891	−3.998025
177	H	−9.389536	−2.889349	−4.278441
178	H	−10.434660	−4.016211	−3.366872
179	C	−7.338105	−0.216616	−1.561051
180	H	−8.296170	−0.735097	−1.617473
181	H	−7.281733	0.359955	−0.635635
182	O	−7.264413	0.786171	−2.638463
183	C	−7.829895	0.423045	−3.866406
184	O	−8.421249	−0.657484	−4.010539
185	C	−7.603138	1.470276	−4.920924
186	H	−6.565215	1.394520	−5.270760
187	H	−7.747345	2.474805	−4.514750
188	H	−8.275902	1.292093	−5.762315
189	O	−2.866377	4.199637	−0.508583
190	C	−3.026054	2.763468	−0.339230
191	H	−2.052681	2.261866	−0.357142
192	C	−3.887749	2.146042	−1.472463
193	H	−4.468022	1.283256	−1.132565
194	C	−4.786225	3.168990	−2.186306
195	H	−5.288293	2.700638	−3.034651
196	C	−4.017936	4.412779	−2.681038
197	H	−4.678042	5.284461	−2.621584
198	C	−2.698762	4.664705	−1.901386
199	H	−1.886142	4.112507	−2.382189
200	O	−2.848159	1.713318	−2.448289

201	C	−3.200703	0.946843	−3.554831
202	O	−4.321792	0.441823	−3.692111
203	C	−2.050975	0.859140	−4.524060
204	H	−1.118580	0.640796	−3.993318
205	H	−1.935670	1.832762	−5.015675
206	H	−2.254619	0.094670	−5.276211
207	O	−5.811249	3.558905	−1.196886
208	C	−7.048075	3.982616	−1.716229
209	O	−7.236810	4.090519	−2.931752
210	C	−8.027634	4.298458	−0.617124
211	H	−7.816282	5.295545	−0.209148
212	H	−7.950050	3.571939	0.196650
213	H	−9.040703	4.303364	−1.024550
214	O	−3.687456	4.179477	−4.102033
215	C	−3.799201	5.272520	−4.982236
216	O	−4.166882	6.386755	−4.593340
217	C	−3.386672	4.891700	−6.377113
218	H	−3.723910	3.881620	−6.625939
219	H	−2.291161	4.920065	−6.441802
220	H	−3.794476	5.612701	−7.088548
221	C	−2.392861	6.162064	−1.826523
222	H	−2.687053	6.647386	−2.761010
223	H	−2.935180	6.606796	−0.988270
224	O	−0.980010	6.486321	−1.554281
225	C	−0.089471	6.372903	−2.613498
226	O	−0.406927	5.812804	−3.681282
227	C	1.236470	7.006124	−2.294589
228	H	1.768827	6.421240	−1.539146
229	H	1.082922	8.014194	−1.895671
230	H	1.852264	7.054148	−3.194892
231	S	−0.209589	−1.588861	1.170474
232	S	0.209652	1.588922	1.170337
233	C	0.406777	4.208481	4.414754
234	C	0.352853	3.024559	3.653879
235	C	0.319109	3.096063	2.250692
236	C	0.339967	4.348644	1.606325
237	C	0.387807	5.522853	2.379028
238	C	0.423688	5.477374	3.791863
239	C	0.473363	6.755325	4.608180
240	H	0.430500	4.146503	5.501290
241	H	0.327976	2.057582	4.149995
242	H	0.314577	4.409687	0.523431
243	H	0.387724	6.484374	1.870141
244	H	1.374071	7.339877	4.378559
245	H	0.474467	6.550313	5.684277
246	H	−0.388620	7.399320	4.390422
247	C	−0.406770	−4.207711	4.415478
248	C	−0.352752	−3.023951	3.654348
249	C	−0.319213	−3.095747	2.251174
250	C	−0.340373	−4.348466	1.607069
251	C	−0.388312	−5.522504	2.380020
252	C	−0.424026	−5.476727	3.792856
253	C	−0.474150	−6.754499	4.609428
254	H	−0.430282	−4.145500	5.502005
255	H	−0.327610	−2.056879	4.150263
256	H	−0.315085	−4.409727	0.524181
257	H	−0.388422	−6.484138	1.871345
258	H	−1.377209	−7.336691	4.382977
259	H	−0.471066	−6.549418	5.685508
260	H	0.385353	−7.400772	4.388726

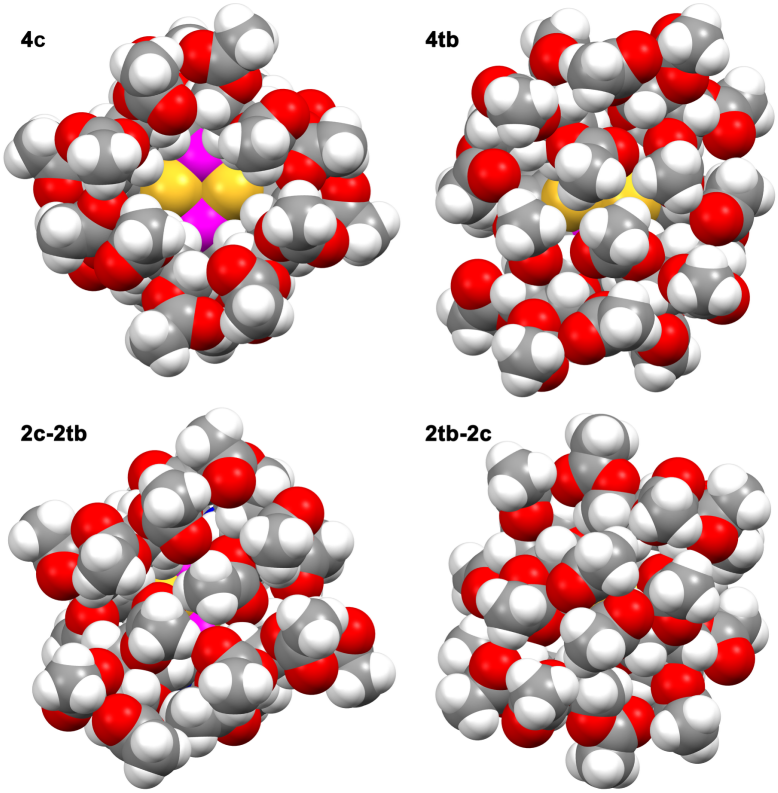

Fig. S23 Space-filling model of isomers of diplatinum complex with bisNHC-C2 ligands $[\mathbf{1}]^{2+}$.

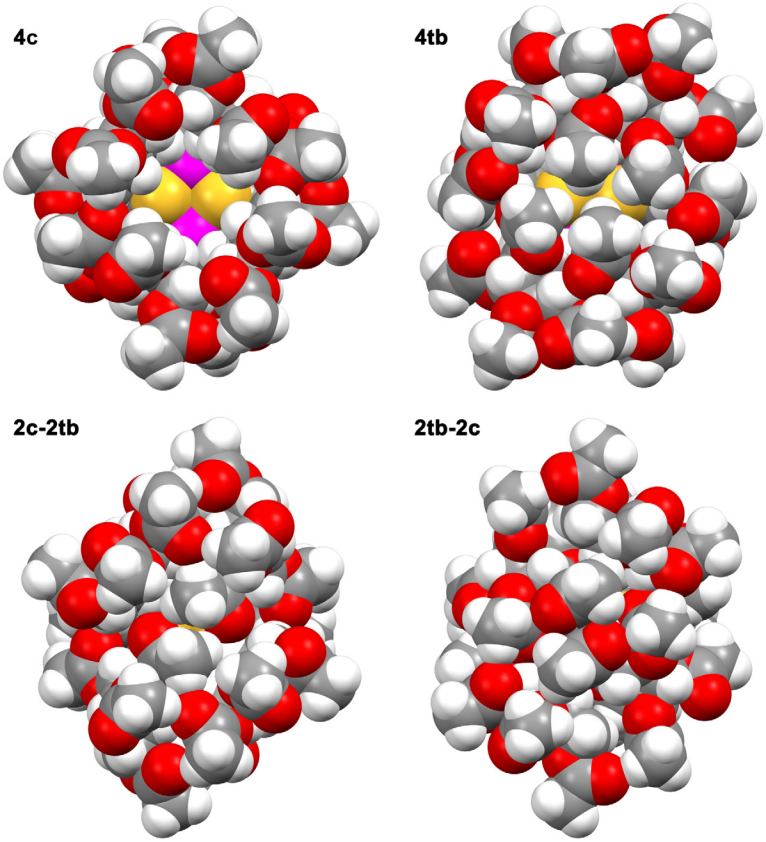

Fig. S24 Space-filling model of isomers of diplatinum complex with bisNHC-C4 ligands $[\mathbf{2}]^{2+}$.

Table S11. Thermodynamic data (Hartree/Particle) obtained from DFT calculations for isomers of [**1**]$^{2+}$.

	4c	**2c–2tb**	**2tb–2c**	**4tb**
Zero–point correction	1.903379	1.902727	1.903625	1.901724
Thermal correction to Energy	2.045695	2.046196	2.046578	2.045796
Thermal correction to Enthalpy	2.046639	2.047140	2.047522	2.046740
Thermal correction to Gibbs Free Energy	1.699649	1.691605	1.698615	1.685876
Sum of electronic and zero–point Energies	–6742.660339	–6742.635998	–6742.625697	–6742.627885
Sum of electronic and thermal Energies	–6742.518023	–6742.492529	–6742.482743	–6742.483814
Sum of electronic and thermal Enthalpies	–6742.517079	–6742.491585	–6742.481799	–6742.482870
Sum of electronic and thermal Free Energies	–6742.864069	–6742.84712	–6742.830706	–6742.843734

Table S12. Thermodynamic data (Hartree/Particle) obtained from DFT calculations for isomers of [**2**]$^{2+}$.

	4c	**2c–2tb**	**2tb–2c**	**4tb**
Zero–point correction	2.066747	2.067836	2.068113	2.066154
Thermal correction to Energy	2.218147	2.219063	2.219256	2.218426
Thermal correction to Enthalpy	2.219091	2.220007	2.220200	2.219370
Thermal correction to Gibbs Free Energy	1.852517	1.85456	1.855821	1.846436
Sum of electronic and zero–point Energies	–7204.520393	–7204.51864	–7204.48432	–7204.49282
Sum of electronic and thermal Energies	–7204.368993	–7204.367413	–7204.333178	–7204.340548
Sum of electronic and thermal Enthalpies	–7204.368049	–7204.366469	–7204.332233	–7204.339604
Sum of electronic and thermal Free Energies	–7204.734623	–7204.731916	–7204.696613	–7204.712538