Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for:

Regulation of Intra- and Intermolecular Pt-Pt and π-π Interactions of a U-Shaped Diplatinum Complex to Achieve Polymorphic Emissions in Solution and Crystalline States

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Table S1. Crystallographic data of different forms of **1**.

compound	**1A**	**1B**	**1C** (solvent squeezed)[a]	**1C** (with disordered solvents)[a]
empirical formula	$C_{35}H_{26}Cl_2N_6OPt_2$ $\cdot CHCl_3 \cdot 1.5(C_2H_4Cl_2)$	$C_{35}H_{26}Cl_2N_6OPt_2$	$C_{35}H_{26}Cl_2N_6OPt_2$	$C_{35}H_{26}Cl_2N_6OPt_2$ $\cdot C_6H_5Cl \cdot C_6H_7Cl$
formula weight	1275.49	1007.70	1007.70	--
space group	P-1	P b c n	P-1	P-1
crystal system	Triclinic	Orthorhombic	Triclinic	Triclinic
a (Å)	11.891(2)	17.353(2)	8.5256(17)	8.5256(17)
b (Å)	14.270(3)	13.8521(17)	16.023(3)	16.023(3)
c (Å)	14.277(3)	25.760(3)	17.850(8)	17.850(8)
α (deg)	64.40(3)	90	66.275(8)	66.28(3)
β (deg)	77.81(3)	90	84.005(11)	84.01(3)
γ (deg)	71.21(3)	90	76.938(10)	76.94(3)
vol ($Å^3$)	2060.9(10)	6192.0(13)	2174.3(11)	2174.4(9)
Z	2	8	2	2
Density (Mg/m^3)	2.055	2.162	1.539	1.439
temp (K)	173.15	173.15	173.15	173.15
wavelength (Å)	0.71073	0.71073	0.71073	0.71073
final R indices	R1 = 0.0322	R1 = 0.0729	R1 = 0.0595	R1 = 0.0721
	wR2 = 0.0591	wR2 = 0.1666	wR2 = 0.1527	wR2 = 0.2234
R indices	R1 = 0.0369	R1 = 0.0839	R1 = 0.0634	R1 = 0.0775
(all data)	wR2 = 0.0609	wR2 = 0.1729	wR2 = 0.1557	wR2 = 0.2286
CCDC No.	1427841	1427838	1427840	1542254

[a]The solvents (PhCl) in crystal **1C** are highly disordered. When solvents were squeezed, high-quality crystallographic data were obtained.

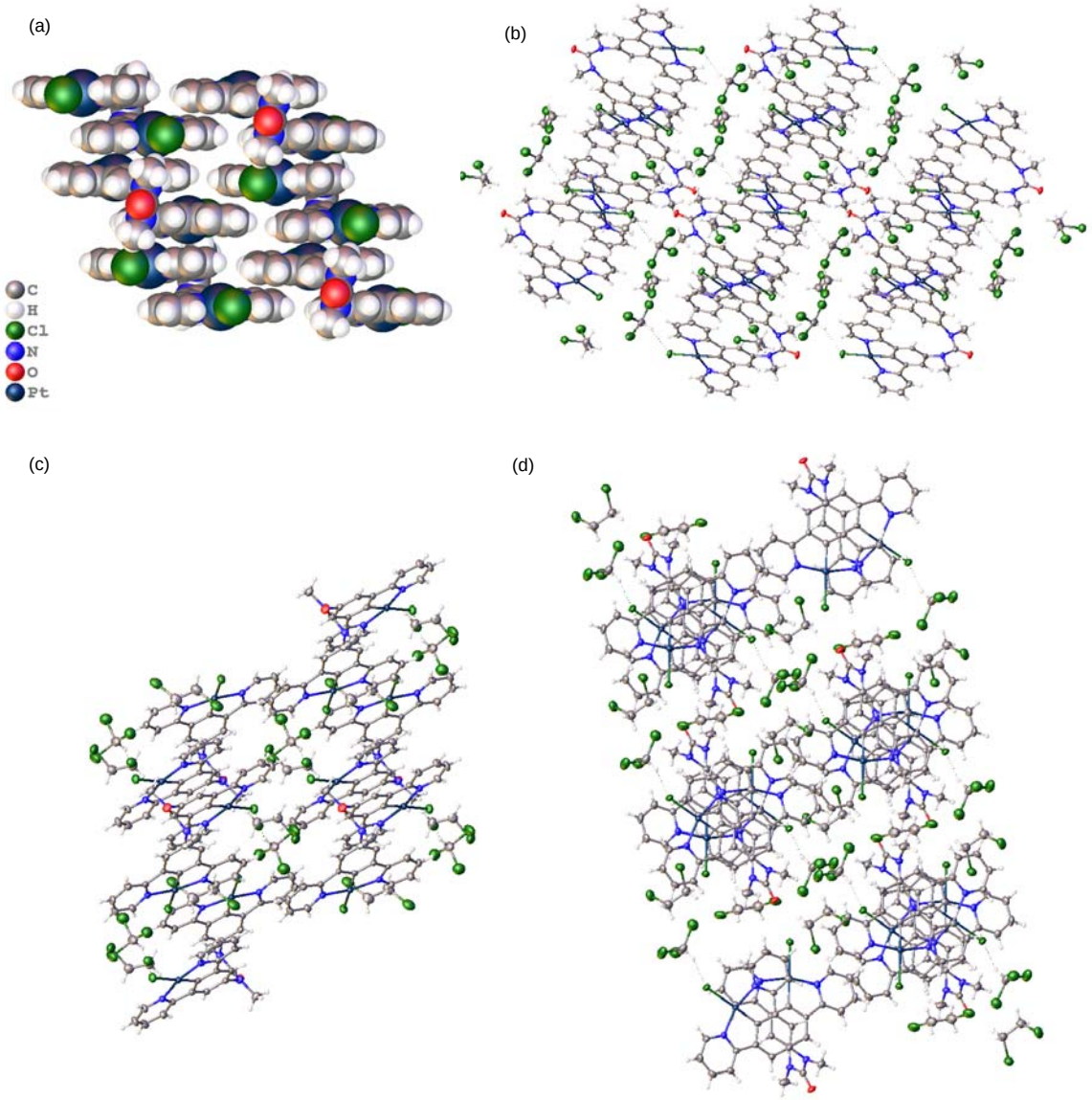

Figure S1. Crystal packing of **1**A. (a) CPK model. (b) View from axis a. (c) View for axis b. (d) View for axis c.

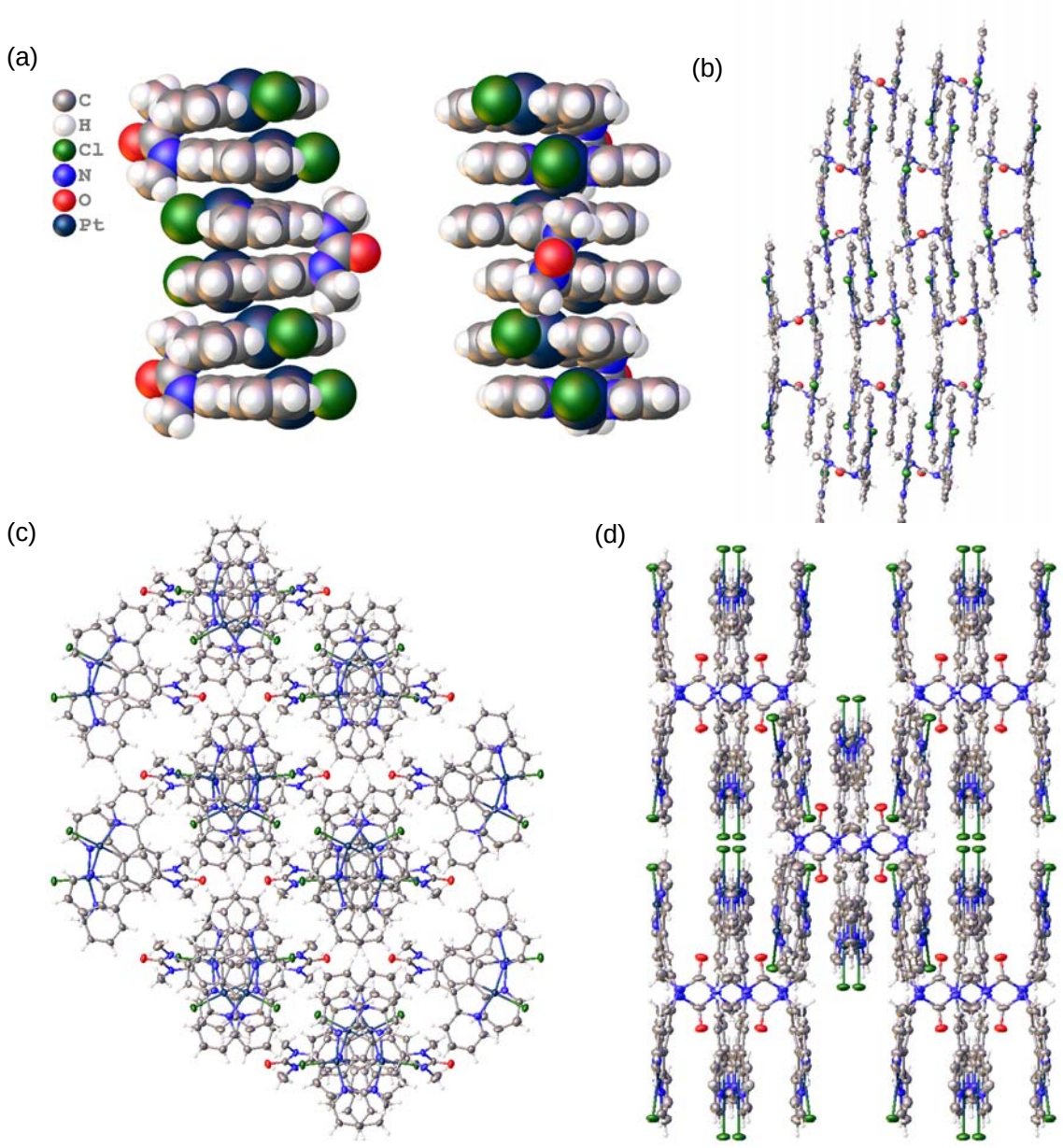

Figure S2. Crystal packing of **1**B. (a) CPK model. (b) View from axis a. (c) View for axis b. (d) View for axis c.

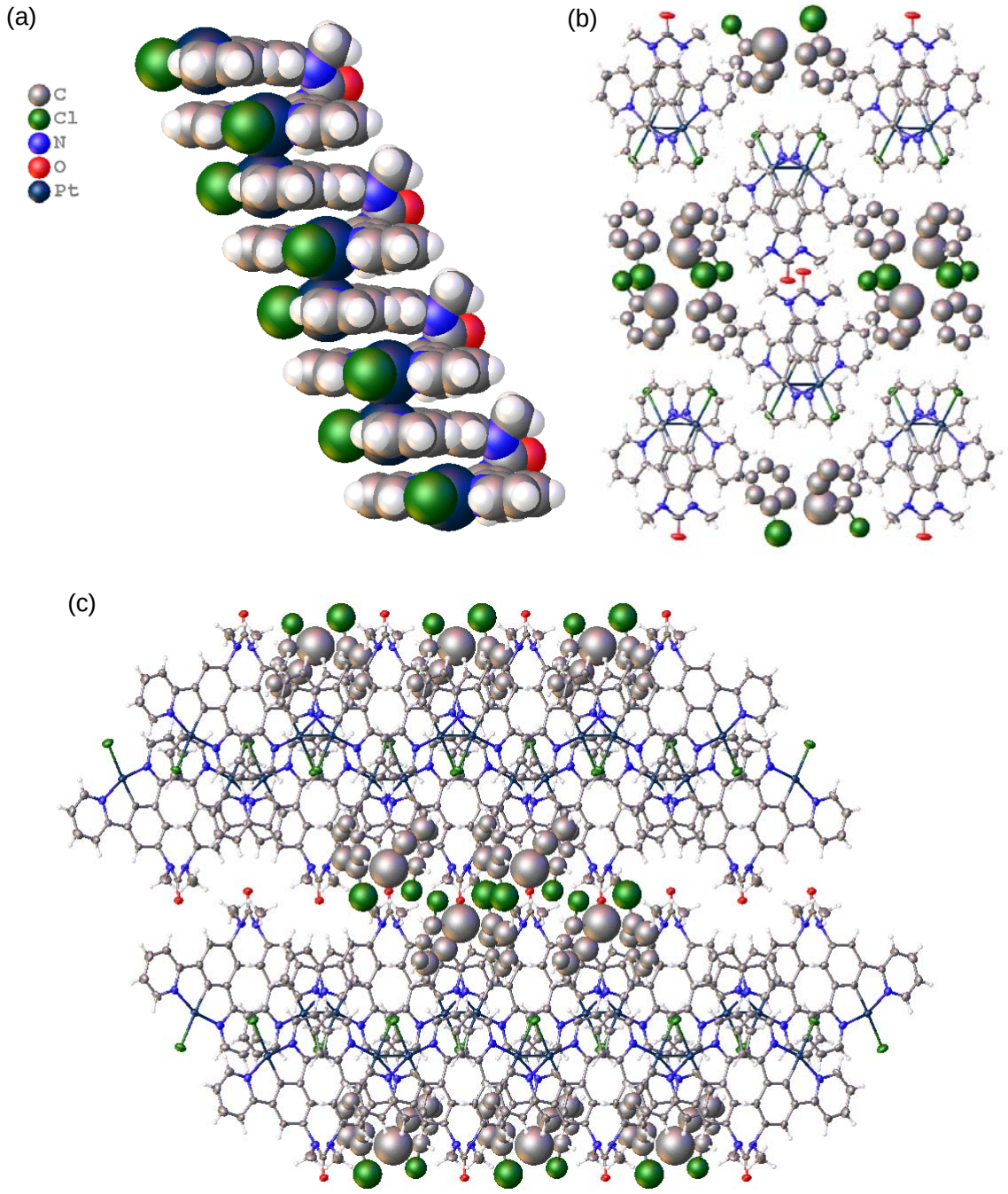

Figure S3. Crystal packing of **1**C (solvents are disordered). (a) CPK model. (b) View from axis a. (c) View for axis b. The PhCl solvents in (b) and (c) are displayed in CPK model.

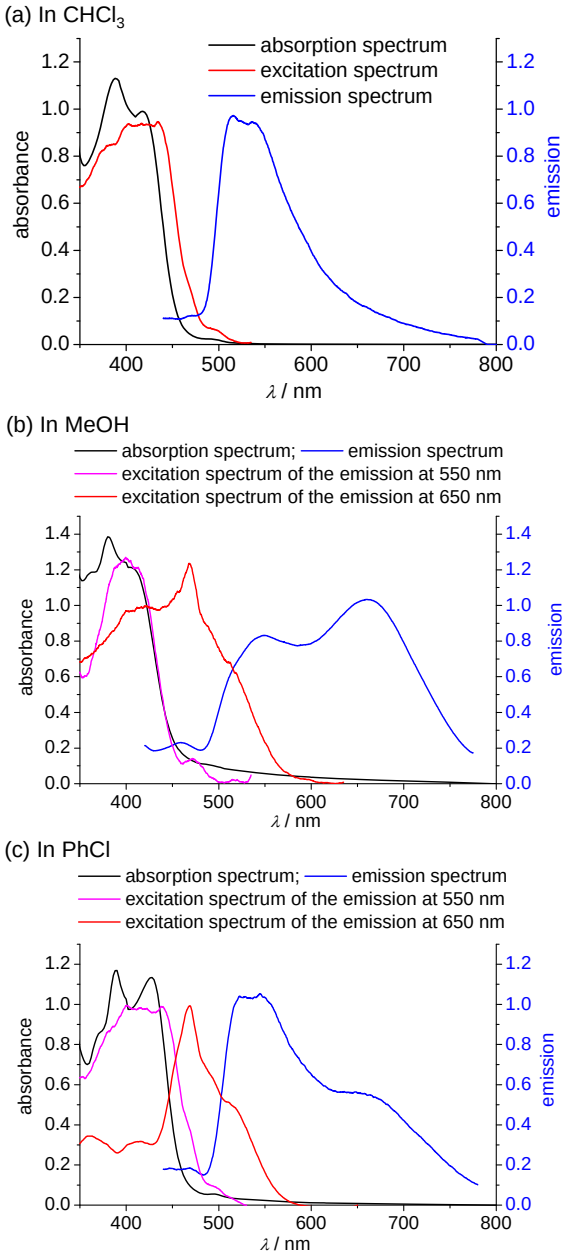

Figure S4. The absorption spectrum, emission spectrum, and excitation spectrum of **1** in different solvents ($CHCl_3$, MeOH, PhCl).

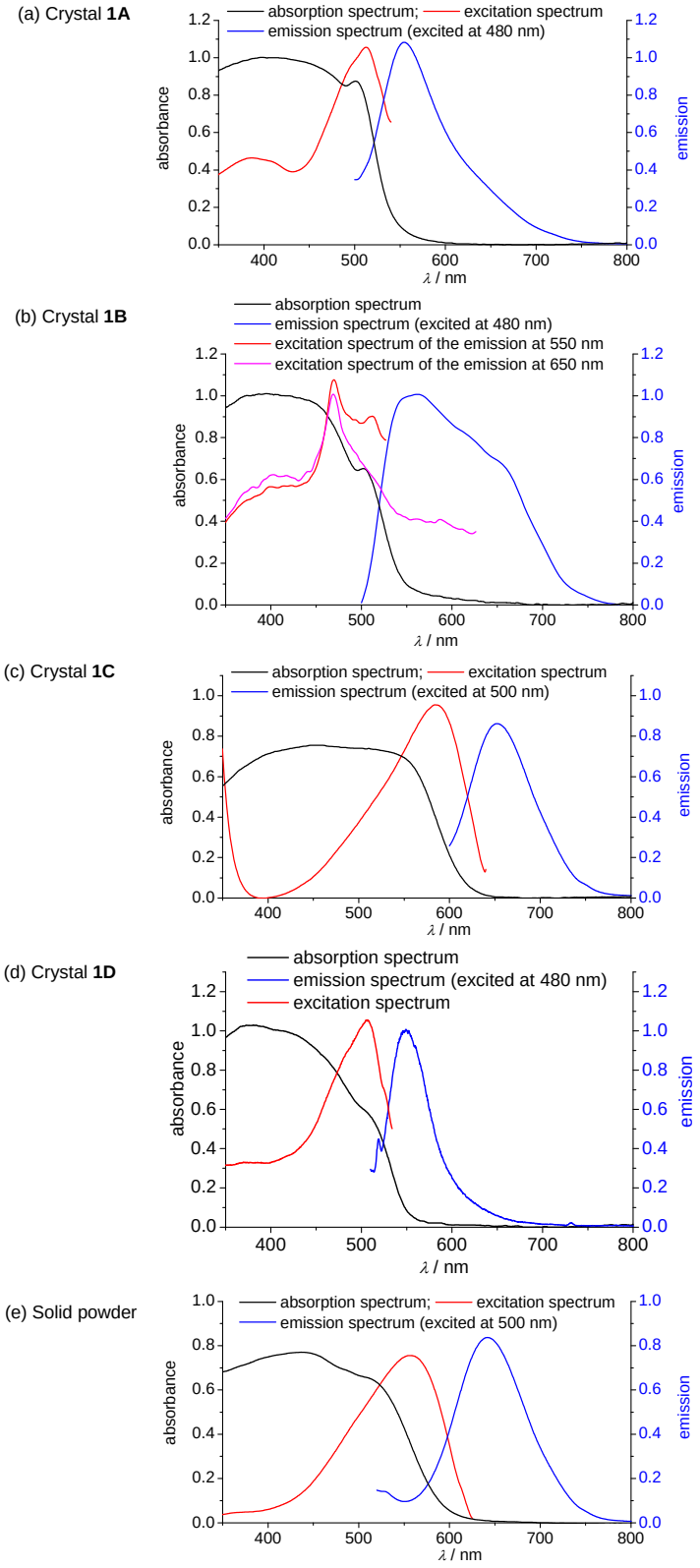

Figure S5. The absorption spectrum, emission spectrum, and excitation spectrum of **1** in different crystal forms and as solid powder.

Cartesian coordinates of the DFT-optimized structure of **1** from the input files generated from **1**B:
Charge = 0; multiplicity=1

Pt	13.45024192	12.02214588	12.48376174
Pt	14.61797142	6.55083392	8.38403641
Cl	15.30818493	12.75854142	13.93465580
Cl	16.95246279	6.26605512	7.62895525
O	6.94250901	8.65620725	9.24479475
N	14.49941805	11.59664636	10.75569332
N	11.88226671	12.21717362	13.81843672
N	8.88516531	9.86281896	9.01664178
N	8.86921146	7.75627429	10.11269291
N	14.93422955	6.95083688	10.38706597
N	13.64826507	6.25726379	6.58113503
C	15.82635783	11.73037495	10.59573881
H	16.35506179	12.12611857	11.45673533
C	16.46219203	11.37106995	9.41141467
H	17.53697028	11.48521639	9.32304287
C	15.69596866	10.85473461	8.36636898
H	16.16531121	10.54203722	7.43885536
C	14.31804895	10.72688354	8.52842354
H	13.70647054	10.31661289	7.73267653
C	13.71918519	11.10307919	9.73156395
C	12.28869568	10.99603420	10.06177373
C	11.24232758	10.49739270	9.27785171
H	11.40243122	10.13581356	8.26613996
C	9.95078689	10.39723850	9.82162796
C	9.67837306	10.82723200	11.13098927
H	8.66146664	10.73669560	11.50506207
C	10.71542172	11.33608212	11.92341410
C	12.00382020	11.40428408	11.37317491
C	10.66328929	11.81901023	13.31114662
C	9.52276960	11.90357218	14.11314734
H	8.56499032	11.59092214	13.71084287
C	9.62143137	12.39081800	15.41396921
H	8.73472953	12.45919231	16.03762158
C	10.86534478	12.79002985	15.90401909
H	10.98226840	13.17586711	16.91079897
C	11.97665309	12.68720849	15.07295728
H	12.97698685	12.97396181	15.38141348
C	8.14108357	10.84176078	8.21742930
H	7.51411707	11.49443614	8.84040300
H	7.49287938	10.31544833	7.51594961
H	8.85697345	11.45950028	7.66856903
C	8.14883311	8.75241342	9.44468585
C	8.06730134	6.65166610	10.64927112
H	7.16142599	7.05203716	11.10574947
H	8.65935114	6.12527868	11.40258346
H	7.77175405	5.93820949	9.86789519
C	10.20966220	7.42296306	9.71600328
C	10.46882094	7.06344612	8.38297086
H	9.63926337	7.04434335	7.68066047
C	11.78027631	6.77323468	7.98559627
C	12.79925769	6.83838910	8.94721409
C	12.55255214	7.16684159	10.28843140
C	11.23832245	7.45555249	10.67249015
H	10.98729415	7.75878328	11.68512453
C	13.78292263	7.22594105	11.09395020

C	13.86639616	7.54924951	12.44908174
H	12.96093452	7.78085801	12.99893781
C	15.10763935	7.58930781	13.08013646
H	15.17510998	7.85580147	14.13040100
C	16.25736741	7.29459281	12.34732715
H	17.24102372	7.31519045	12.80329706
C	16.13013748	6.97986638	10.99803968
H	16.97791092	6.74783645	10.36180939
C	12.28043226	6.41886537	6.64923474
C	11.50786449	6.24111367	5.49915060
H	10.43172509	6.36608893	5.55616606
C	12.11996074	5.90075104	4.29543218
H	11.51975166	5.76002524	3.40114409
C	13.50545675	5.74140789	4.25181843
H	14.01831078	5.47580213	3.33391552
C	14.23790119	5.92893063	5.41995425
H	15.31737409	5.82613753	5.46669251

Cartesian coordinates of the DFT-optimized structure of **1** from the input files generated from **1**C:
Charge = 0; multiplicity=1

Pt	11.65660653	6.47744989	9.39754314
Pt	4.96974396	8.29603175	9.42850652
Cl	12.56084742	5.61352194	7.26835551
Cl	4.04988899	9.11761213	7.28892114
O	8.36743639	7.46778315	16.63196383
N	12.53543114	5.13506219	10.70285249
N	10.51048058	8.04347222	8.68871662
N	9.11806474	8.35001122	14.64794889
N	7.57927926	6.54099080	14.68346383
N	4.14427708	9.69705376	10.70687540
N	6.06823866	6.68363365	8.74848433
C	13.39171147	4.15816977	10.36184310
H	13.61302716	4.09115538	9.30137608
C	13.94417289	3.30192937	11.30942159
H	14.63283326	2.52572576	10.99413980
C	13.59405933	3.46847139	12.64974755
H	14.00857075	2.81698917	13.41367048
C	12.70668856	4.48154113	13.00416894
H	12.42346909	4.63092795	14.04071932
C	12.17627309	5.32046549	12.02132115
C	11.23825964	6.43105729	12.24117361
C	10.64416144	6.85504913	13.43685749
H	10.84268938	6.35907209	14.38378514
C	9.74428230	7.93368541	13.42182769
C	9.45444822	8.62154064	12.23157751
H	8.73794344	9.43694224	12.27258462
C	10.03749084	8.20492849	11.02972787
C	10.91647208	7.11218668	11.05805457
C	9.81086386	8.71606376	9.66818275
C	8.95671537	9.76056164	9.31154136
H	8.38869047	10.27205051	10.08057920
C	8.81916341	10.12175941	7.97306778
H	8.14004607	10.92098120	7.69297183
C	9.55031312	9.43771743	7.00182803
H	9.47055103	9.69018107	5.95022562
C	10.38703183	8.39953337	7.39938112
H	10.97794750	7.81477071	6.70194884
C	9.84045767	9.36775157	15.41820083
H	10.74499108	8.96319705	15.89281064
H	9.18942635	9.75622313	16.20222502
H	10.12808382	10.17662376	14.74142382
C	8.35581116	7.45384351	15.40555635
C	6.87176521	5.54102080	15.48997367
H	7.53735763	5.17034539	16.27034718
H	6.57177542	4.71692278	14.83736694
H	5.97603937	5.95651998	15.97174589
C	6.93208178	6.92828277	13.45933583
C	6.05239837	8.02352478	13.45792499
H	5.88329174	8.55362047	14.39190685
C	5.44241809	8.42116386	12.26118508
C	5.72637608	7.69618526	11.09457499
C	6.58250629	6.58512884	11.08423540
C	7.18263763	6.19591923	12.28682176
H	7.88416066	5.36821050	12.34001524
C	4.52390437	9.54448100	12.02380628

C	4.02988354	10.42473592	12.98933996
H	4.32900722	10.30118949	14.02482056
C	3.15789695	11.44561218	12.61936733
H	2.77170972	12.12930342	13.36986428
C	2.78642038	11.57831656	11.28099308
H	2.10870147	12.35930947	10.95404785
C	3.30275520	10.68135466	10.35088453
H	3.06354102	10.72029026	9.29291146
C	6.77111416	6.02619918	9.73576699
C	7.59316895	4.95036538	9.39719732
H	8.16271729	4.44954682	10.17215936
C	7.69470780	4.54266822	8.06891639
H	8.34724177	3.71710268	7.80213274
C	6.96148827	5.21326419	7.08984735
H	7.01414596	4.92520101	6.04572259
C	6.15802538	6.28396258	7.46926310
H	5.56776758	6.86067471	6.76463592