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Metal-metal bond formation of triplatinum cores with a silver(I) ion affording a heptanuclear cluster bearing four Pt–Ag bonds

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Supplementary Information

1. Experimental Procedures
2. X-ray crystallography
3. DFT calculations
4. References

1. Experimental Procedures

General Procedures: All chemicals were purchased from Sigma-Aldrich, Nacalai Tesque and Wako Pure Chemical Industries. All reagents and solvents were used as received. *cis*-[Pt(bisNHC-C1)$(SH)_2$] (bisNHC-C1 = 1,1'-Dimethyl-3,3'-methylene-4-diimidazolilydene) was prepared according to the reported procedures.[1] *cis*-[Pt(bisNHC-C1)Cl_2] was synthesised from the reaction of $K_2[PtCl_4]$ and [(bisNHC-C1)H_2]$(PF_6)_2$ in DMSO using a previously reported procedure.[1] ^{1}H NMR spectra were recorded on a Bruker AVANCE 300 FT-NMR spectrometer. Chemical shifts (δ in ppm, coupling constants J in Hz) for ^{1}H NMR signals are expressed from $SiMe_4$ and referenced to residual solvent resonances.

Synthesis of [{Pt(bisNHC-C1)}$_3$(μ_3-S)$_2$](OTf)$_2$

A mixture of *cis*-[Pt(bisNHC-C1)$(SH)_2$] (0.11 g, 0.25 mmol), *cis*-[Pt(bisNHC-C1)Cl_2] (0.22 g, 0.50 mmol) and $KHCO_3$ (1.1 g, 11 mmol) as a proton scavenger in DMSO (30 mL) was stirred for 20 min to give a yellow mixture, which was heated at 60 ºC for 4 h to afford a pale-yellow mixture. The solvent was removed under reduced pressure to give a pale-yellow solid. The solid was re-dissolved in water and added a solution of NaOTf (0.86 g 5.0 mmol) in water (3 mL) to give a slightly hygroscopic white solid, which was collected by suction filtration and washed with water. Yield: 0.20 g, 54%. The product was purified by recrystallisation from a solution in CH_3CN by the addition of Et_2O. Single crystals suitable for X-ray crystallography were obtained from a solution of a crude product, which contained a small amount of Cl^- as counter anions, in CH_3CN by diffusion of MeOH as [{Pt(bisNHC-C1)}$_3$(μ_3-S)$_2$]Cl(OTf). Anal. Calcd for [{Pt(bisNHC-C1)}$_3$(μ_3-S)$_2$](OTf)$_2$•0.5H_2O ($C_{29}H_{37}F_6N_{12}O_{6.5}Pt_3S_4$): C, 23.45; H, 2.51; N, 11.32. Found: C, 23.60; H, 32.75; N, 11.21. ^{1}H NMR (CD_3CN, 300 MHz, 243 K): C_s isomer: δ 7.24 (d, $^3J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 7.20 (d, $^3J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 7.16 (d, $^3J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 7.09 (d, $^3J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 7.04 (d, $^3J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 6.94 (d, $^3J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 5.82–5.69 (N-CH_2), 3.94 (s, 6H, N-Me), 3.88 (s, 6H, N-Me), 3.57 (s, 6H, N-Me). C_{3h} isomer: δ 7.20 (d, $^3J_{H\text{-}H}$ = 2.0

Hz, 6H, im), 6.99 (d, $^{3}J_{H\text{-}H}$ = 2.0 Hz, 6H, im), 5.82–5.69 (N-CH_2), 3.74 (s, 18H, N-Me).

Synthesis of [Ag{[Pt(bisNHC-C1)]$_3$(μ_3-S)$_2$}$_2$](OTf)$_4$(PF_6)

A solution of AgOTf (0.069 g, 0.027 mmol) in CH_3CN (1 mL) was added to a solution of [{Pt(bisNHC-C1)}$_3$(μ_3-S)$_2$](OTf)$_2$ (0.074 g, 0.050 mmol) in CH_3CN (2 mL). The solution was stirred for 30 min to give a white solid. The white solid was removed by filtration using a membrane filter. Diethyl ether was added to the filtrate to afford a yellow solid, which was collected by suction filtration and washed with diethyl ether. Yield: 0.034 g, 43%. The pure sample used for elemental analysis was obtained from a crude product, which contains a small amount of PF_6^- as impurity originated from the ligand precursor used as a starting material to prepare the chloro complex, by recrystallisation three times from a solution in CH_3CN by the addition of Et_2O. Repeated recrystallisation probably concentrates PF_6^- anions due to low solubility of the salt containing PF_6^- ions. A few number of single crystals suitable for X-ray crystallography were obtained from a solution of a crude product in CH_3CN by diffusion of Et_2O as [Ag{[Pt(bisNHC-C1)]$_3$(μ_3-S)$_2$}$_2$](OTf)$_3$(PF_6)$_2$. Anal. Calcd for $C_{58}H_{72}AgF_{18}N_{24}O_{12}PPt_6S_8$: C, 21.73; H, 2.26; N, 10.49. Found: C, 21.91; H, 2.42; N, 10.41. ^{1}H NMR (CD_3CN, 300 MHz, 298 K): δ 7.35 (dd, $^{3}J_{H\text{-}H}$ = 2.0 Hz, $^{3}J_{H\text{-}H}$ = 2.0 Hz, 4H, im), 7.20 (t, $^{3}J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 7.04 (t, $^{3}J_{H\text{–}H}$ = 1.6 Hz, 2H, im), 6.99 (d, $^{3}J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 6.98 (d, $^{3}J_{H\text{-}H}$ = 1.9 Hz, 2H, im), 8.39 (d, $^{3}J_{H\text{-}H}$ = 1.9 Hz, 2H, im), 6.84 (d, $^{3}J_{H\text{-}H}$ = 1.9 Hz, 2H, im), 6.77 (d, $^{3}J_{H\text{-}H}$ = 2.0 Hz, 2H, im), 6.34 (d, $^{2}J_{H\text{-}H}$ = 13.1 Hz, 2H, N-CH_2), 6.18 (d, $^{2}J_{H\text{-}H}$ = 13.2 Hz, 2H, N-CH_2), 5.90–5.79 (N-CH_2), 4.06 (s, 6H, N-Me), 4.01 (s, 6H, N-Me), 3.95 (s, 6H, N-Me), 3.94 (s, 6H, N-Me), 3.49 (s, 6H, N-Me), 3.46 (s, 6H, N-Me).

2. X-ray crystallography

Each single crystal of [**1**]Cl(OTf) and [**2**](OTf)$_3$(PF_6)$_2$ was mounted on a loop using Paratone. Diffraction data were collected on a Rigaku Varimax Saturn724 diffractometer using a rotation method with 0.5° frame widths.

The data were integrated, scaled, sorted, and averaged using the CrystalClear[2] software. Absorption corrections were applied using the multi-scan method. The structures were solved using SIR97[3] and refined with SHELXL97[4] using the CrystalStructure software.[5] All hydrogen atoms were located at the calculated positions and refined as ridding models. Crystallographic data are summarised in Tables S1 and S2 for [**1**]Cl(OTf) and [**2**](OTf)$_3$(PF$_6$)$_2$, respectively.

Table S1. Crystallographic data of triplatinum complex [**1**]Cl(OTf).

Formula	$C_{28}H_{36}ClF_3N_{12}O_3Pt_3S_3$
M_w	1362.57
Crystal description	colourless, prism
Crystal size/mm	0.126 × 0.096 × 0.091
Crystal system	*monoclinic*
Space group	*C*2/*c* (#15)
a/Å	38.466(7)
b/Å	18.519(3)
c/Å	28.967(5)
β/°	113.9235(16)
V/Å^3	18862(6)
Z	16
F(000)	10208.00
ρ_{calcd}/g cm^{-1}	1.919
μ/mm^{-1}	9.084
Total reflections	95400
Unique reflections (R_{int})	21456 (0.0401)
Scan range θ/°	27.450
Completeness	0.995
Index ranges	$-49 \le h \le 49$
	$-23 \le k \le 23$
	$-37 \le l \le 37$
Data/restrains/para.	21456/0/974
R1 [I>2σ(*I*)], *wR*2 (all data)	0.0651, 0.1813
GOF on F^2	1.095

Max./min. ρ/eÅ^{-3}	2.94/–2.41
Min./max. T	0.350/0.438

Table S2. Crystallographic data of heptanuclear cluster [**2**](OTf)$_3$(PF$_6$)$_2$.

Formula	$C_{57}H_{72}F_{21}N_{14}O_9P_2Pt_6S_7$
M_w	3201.09
Crystal description	yellow, prism
Crystal size/mm	0.090 × 0.060 × 0.060
Crystal system	*monoclinic*
Space group	*C*2/*c* (#15)
a/Å	22.410(3)
b/Å	22.131(3)
c/Å	18.447(3)
β/°	108.832(2)
V/Å^3	8659(2)
Z	4
F(000)	6000.00
ρ_{calcd}/g cm^{-1}	2.455
μ/mm^{-1}	10.153
Total reflections	35559
Unique reflections (R_{int})	9844 (0.0261)
Scan range θ/°	27.48
Completeness	0.989
Index ranges	$-28 \leq h \leq 28$
	$-28 \leq k \leq 28$
	$-23 \leq l \leq 23$
Data/restrains/para.	9844/0/578
R1 [I>2σ(*I*)], *wR*2 (all data)	0.0377, 0.0952
GOF on F^2	1.054
Max./min. ρ/eÅ^{-3}	3.64/–1.55
Min./max. T	0.403/0.544

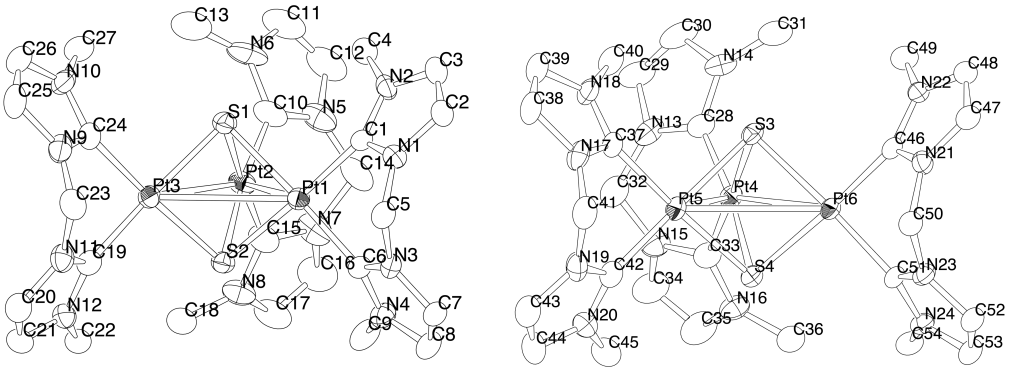

Fig. S-1 Atom numbering for [**1**]Cl(OTf)

Table S3. Selected bond distances for [**1**]Cl(OTf).

Atoms	Distance/Å	Atoms	Distance/Å
Pt1–Pt2	2.9734(9)	Pt1–Pt3	3.1824(7)
Pt1–S1	2.376(3)	Pt1–S2	2.372(3)
Pt1–C1	2.030(11)	Pt1–C6	2.025(12)
Pt2–Pt3	3.3233(8)	Pt2–S1	2.375(3)
Pt2–S2	2.370(3)	Pt2–C10	1.992(19)
Pt2–C15	1.986(13)	Pt3–S1	2.354(3)
Pt3–S2	2.349(2)	Pt3–C19	2.023(13)
Pt3–C24	2.009(11)	Pt4–Pt5	2.9525(8)
Pt4–Pt6	3.3184(8)	Pt4–S3	2.374(3)
Pt4–S4	2.377(3)	Pt4–C28	2.007(14)
Pt4–C33	2.009(13)	Pt5–Pt6	3.2391(6)
Pt5–S3	2.368(3)	Pt5–S4	2.382(2)
Pt5–C37	2.002(9)	Pt5–C42	2.016(13)
Pt6–S3	2.351(3)	Pt6–S4	2.360(3)
Pt6–C46	2.011(11)	Pt6–C51	2.036(9)

Table S4. Selected bond angles for [**1**]Cl(OTf).

Atoms	Angle/°	Atoms	Angle/°
Pt2–Pt1–Pt3	65.247(18)	Pt2–Pt1–S1	51.24(8)
Pt2–Pt1–S2	51.13(8)	Pt2–Pt1–C1	125.8(4)
Pt2–Pt1–C6	125.4(4)	Pt3–Pt1–S1	47.42(7)
Pt3–Pt1–S2	47.30(6)	Pt3–Pt1–C1	131.3(3)
Pt3–Pt1–C6	131.0(3)	S1–Pt1–S2	78.27(10)
S1–Pt1–C1	98.7(3)	S1–Pt1–C6	176.3(4)
S2–Pt1–C1	176.7(4)	S2–Pt1–C6	98.3(3)
C1–Pt1–C6	84.6(5)	Pt1–Pt2–Pt3	60.413(19)

Pt1–Pt2–S1	51.26(9)	Pt1–Pt2–S2	51.20(7)
Pt1–Pt2–C10	120.5(5)	Pt1–Pt2–C15	122.3(5)
Pt3–Pt2–S1	45.09(7)	Pt3–Pt2–S2	44.96(6)
Pt3–Pt2–C10	136.5(4)	Pt3–Pt2–C15	134.1(4)
S1–Pt2–S2	78.33(11)	S1–Pt2–C10	98.4(4)
S1–Pt2–C15	173.5(5)	S2–Pt2–C10	171.3(5)
S2–Pt2–C15	97.5(5)	C10–Pt2–C15	85.1(6)
Pt1–Pt3–Pt2	54.340(14)	Pt1–Pt3–S1	48.00(8)
Pt1–Pt3–S2	47.93(7)	Pt1–Pt3–C19	128.3(4)
Pt1–Pt3–C24	129.5(4)	Pt2–Pt3–S1	45.61(7)
Pt2–Pt3–S2	45.49(8)	Pt2–Pt3–C19	135.1(3)
Pt2–Pt3–C24	131.4(4)	S1–Pt3–S2	79.17(9)
S1–Pt3–C19	176.0(4)	S1–Pt3–C24	97.2(4)
S2–Pt3–C19	99.2(3)	S2–Pt3–C24	176.4(4)
C19–Pt3–C24	84.4(5)	Pt5–Pt4–Pt6	61.873(15)
Pt5–Pt4–S3	51.39(7)	Pt5–Pt4–S4	51.72(5)
Pt5–Pt4–C28	119.1(3)	Pt5–Pt4–C33	122.7(4)
Pt6–Pt4–S3	45.10(6)	Pt6–Pt4–S4	45.32(7)
Pt6–Pt4–C28	135.8(4)	Pt6–Pt4–C33	133.8(4)
S3–Pt4–S4	77.97(9)	S3–Pt4–C28	97.9(3)
S3–Pt4–C33	174.1(4)	S4–Pt4–C28	170.6(3)
S4–Pt4–C33	97.8(4)	C28–Pt4–C33	85.6(5)
Pt4–Pt5–Pt6	64.624(14)	Pt4–Pt5–S3	51.59(7)
Pt4–Pt5–S4	51.58(8)	Pt4–Pt5–C37	121.0(4)
Pt4–Pt5–C42	126.1(4)	Pt6–Pt5–S3	46.43(6)
Pt6–Pt5–S4	46.63(6)	Pt6–Pt5–C37	132.5(3)
Pt6–Pt5–C42	133.0(3)	S3–Pt5–S4	78.01(8)
S3–Pt5–C37	96.9(3)	S3–Pt5–C42	177.7(4)
S4–Pt5–C37	172.6(4)	S4–Pt5–C42	100.1(3)
C37–Pt5–C42	84.8(4)	Pt4–Pt6–Pt5	53.503(16)
Pt4–Pt6–S3	45.67(7)	Pt4–Pt6–S4	45.74(7)
Pt4–Pt6–C46	134.0(3)	Pt4–Pt6–C51	132.4(3)
Pt5–Pt6–S3	46.87(7)	Pt5–Pt6–S4	47.19(5)
Pt5–Pt6–C46	128.6(2)	Pt5–Pt6–C51	130.5(3)
S3–Pt6–S4	78.77(9)	S3–Pt6–C46	98.6(3)
S3–Pt6–C51	177.0(3)	S4–Pt6–C46	175.8(2)
S4–Pt6–C51	98.4(3)	C46–Pt6–C51	84.3(4)
Pt1–S1–Pt2	77.50(8)	Pt1–S1–Pt3	84.58(11)
Pt2–S1–Pt3	89.30(10)	Pt1–S2–Pt2	77.66(8)
Pt1–S2–Pt3	84.77(8)	Pt2–S2–Pt3	89.55(10)
Pt4–S3–Pt5	77.02(8)	Pt4–S3–Pt6	89.22(7)
Pt5–S3–Pt6	86.70(9)	Pt4–S4–Pt5	76.70(7)
Pt4–S4–Pt6	88.95(9)	Pt5–S4–Pt6	86.18(8)

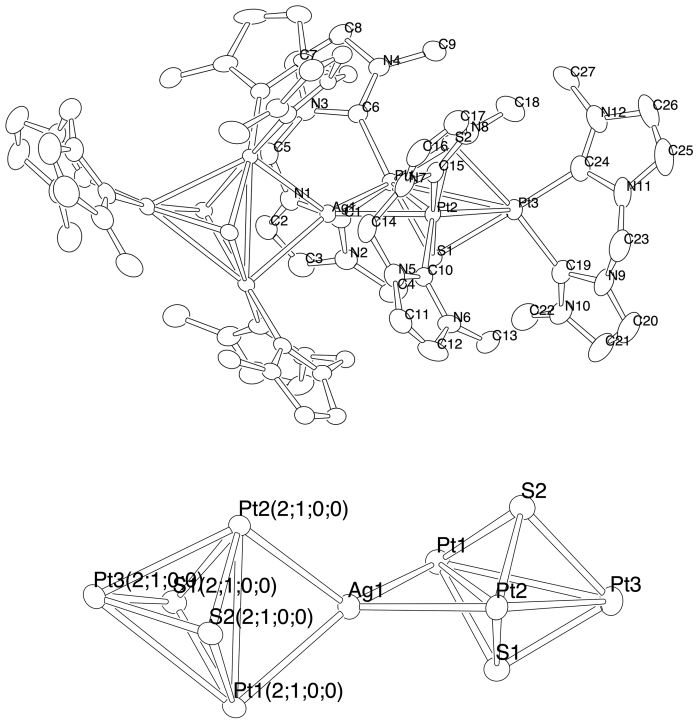

Fig. S-2 Atom numbering for [**2**](OTf)$_3$(PF$_6$)$_2$

Table S5. Selected bond distances for [**2**](OTf)$_3$(PF$_6$)$_2$.

Atoms	Distance/Å	Atoms	Distance/Å
Pt1–Ag1	2.8138(4)	Pt1–S1	2.3580(19)
Pt1–S2	2.3544(16)	Pt1–C1	2.027(7)
Pt1–C6	2.035(7)	Pt2–Pt3	2.9109(5)
Pt2–Ag1	2.7741(5)	Pt2–S1	2.3908(16)
Pt2–S2	2.3691(15)	Pt2–C10	2.004(6)
Pt2–C15	2.019(7)	Pt3–S1	2.3816(16)
Pt3–S2	2.3733(18)	Pt3–C19	2.007(9)

Table S6. Selected bond angles for [**2**](OTf)$_3$(PF$_6$)$_2$.

Atoms	Angle/°	Atoms	Angle/°
Ag1–Pt1–S1	74.44(4)	Ag1–Pt1–S2	88.85(4)
Ag1–Pt1–C1	90.36(18)	Ag1–Pt1–C6	105.78(18)
S1–Pt1–S2	78.45(6)	S1–Pt1–C1	98.8(2)
S1–Pt1–C6	175.81(19)	S2–Pt1–C1	177.3(2)
S2–Pt1–C6	97.36(19)	C1–Pt1–C6	85.4(3)
Pt3–Pt2–Ag1	117.362(16)	Pt3–Pt2–S1	52.27(4)
Pt3–Pt2–S2	52.20(4)	Pt3–Pt2–C10	122.4(2)
Pt3–Pt2–C15	124.38(18)	Ag1–Pt2–S1	74.73(5)

Ag1–Pt2–S2	89.51(4)	Ag1–Pt2–C10	94.2(2)
Ag1–Pt2–C15	106.2(2)	S1–Pt2–S2	77.52(5)
S1–Pt2–C10	99.7(2)	S1–Pt2–C15	175.56(18)
S2–Pt2–C10	174.6(2)	S2–Pt2–C15	98.11(18)
C10–Pt2–C15	84.6(3)	Pt2–Pt3–S1	52.56(4)
Pt2–Pt3–S2	52.07(3)	Pt2–Pt3–C19	119.97(19)
Pt2–Pt3–C24	118.4(2)	S1–Pt3–S2	77.61(6)
S1–Pt3–C19	96.5(2)	S1–Pt3–C24	170.6(2)
S2–Pt3–C19	171.96(19)	S2–Pt3–C24	98.7(3)
C19–Pt3–C24	86.3(3)	Pt1–Ag1–Pt1*	141.66(3)
Pt1–Ag1–Pt2	72.283(12)	Pt1–Ag1–Pt2*	128.381(12)
Pt1*–Ag1–Pt2	128.381(12)	Pt2–Ag1–Pt2*	122.36(3)
Pt1–S1–Pt2	87.90(6)	Pt1–S1–Pt3	89.14(5)
Pt2–S1–Pt3	75.17(5)	Pt1–S2–Pt2	88.49(5)
Pt1–S2–Pt3	89.42(6)	Pt2–S2–Pt3	75.73(5)

3. DFT calculations

DFT calculations were carried out on triplatinum complex cation [**1**]$^{2+}$ and heptanuclear cluster [**2**]$^{5+}$ using Gaussian03.[6] Atomic coordinates were optimised at the level of B3LYP/LanL2DZ. Structural optimisations were started from the structures obtained from crystallographic analyses. Vibrational frequencies were calculated for all converged structures, and no imaginary frequencies appeared showing that these structures lie on minima.

Table S7. Optimised atomic coordinates of triplatinum complex [**1**]$^{2+}$ obtained from DFT calculations

Number	Atom	x	y	z
1	Pt	–0.162053	1.733422	–0.007849
2	Pt	1.853510	–0.835834	–0.001239
3	Pt	–1.664627	–1.161456	0.006396
4	S	0.016195	–0.214267	–1.576693
5	S	0.023400	–0.202551	1.575928
6	N	–1.285436	4.217501	–1.220668
7	N	0.214746	3.444567	–2.597702
8	N	–1.278672	4.232287	1.179655
9	N	0.229127	3.477597	2.558395
10	N	4.594441	–0.714891	–1.177468
11	N	3.364606	–1.878087	–2.547151
12	N	4.573961	–0.695601	1.219177
13	N	3.320383	–1.856946	2.568853
14	N	–4.366770	–1.534432	–1.206722
15	N	–2.920858	–2.454716	–2.549078
16	N	–4.382148	–1.507042	1.191386
17	N	–2.957342	–2.393146	2.578614

18	C	–0.391025	3.174200	–1.394957
19	C	–1.239781	5.117943	–2.297957
20	H	–1.857805	5.998772	–2.361305
21	C	–0.301067	4.625290	–3.164269
22	H	0.039509	5.008874	–4.112253
23	C	1.279812	2.648504	–3.231067
24	H	0.881893	2.098892	–4.089751
25	H	1.667566	1.933433	–2.506272
26	H	2.082721	3.315332	–3.561913
27	C	–2.117542	4.318075	–0.018684
28	H	–2.651922	5.270399	–0.023004
29	H	–2.838196	3.494792	–0.011590
30	C	–0.384044	3.190507	1.363143
31	C	–1.225407	5.148051	2.243586
32	H	–1.842590	6.030058	2.298295
33	C	–0.281910	4.667001	3.111056
34	H	0.064888	5.063707	4.051369
35	C	1.300372	2.693198	3.195302
36	H	2.126924	3.358660	3.465651
37	H	1.648898	1.934984	2.495054
38	H	0.921124	2.196523	4.093878
39	C	3.302487	–1.181229	–1.364834
40	C	4.665405	–1.843645	–3.084284
41	H	4.922395	–2.332719	–4.009854
42	C	5.442805	–1.117409	–2.222547
43	H	6.487995	–0.858216	–2.271048
44	C	2.261271	–2.636424	–3.157477
45	H	2.467248	–3.710721	–3.096835
46	H	2.147701	–2.346183	–4.206820
47	H	1.343901	–2.403511	–2.618991
48	C	4.963234	0.049560	0.017850
49	H	4.440054	1.010554	0.005968
50	H	6.041705	0.220231	0.025563
51	C	3.282615	–1.169429	1.380673
52	C	5.399229	–1.079314	2.289558
53	H	6.441998	–0.815322	2.358957
54	C	4.605942	–1.802534	3.139908
55	H	4.844460	–2.279498	4.076594
56	C	2.194856	–2.591223	3.168881
57	H	1.462999	–2.803620	2.389574
58	H	1.720698	–1.991568	3.952048
59	H	2.560938	–3.530962	3.593408
60	C	–3.027969	–1.733233	1.376640
61	C	–5.138005	–2.012262	2.262601
62	H	–6.212034	–1.939047	2.316882
63	C	–4.238582	–2.562469	3.135827
64	H	–4.398453	–3.055437	4.080920
65	C	–1.728616	–2.900746	3.207843
66	H	–0.922500	–2.854602	2.476576

67	H	–1.881608	–3.937523	3.524270
68	H	–1.463344	–2.286202	4.074043
69	C	–4.891115	–0.855303	–0.018637
70	H	–5.982276	–0.897754	–0.024970
71	H	–4.565928	0.189247	–0.028619
72	C	–3.010569	–1.764390	–1.365950
73	C	–5.106360	–2.066645	–2.276209
74	H	–6.179500	–1.996245	–2.348290
75	C	–4.193389	–2.638006	–3.121669
76	H	–4.338883	–3.154413	–4.056444
77	C	–1.679031	–2.968853	–3.147659
78	H	–0.923009	–3.047266	–2.366142
79	H	–1.321447	–2.289576	–3.927807
80	H	–1.866315	–3.958236	–3.576027

Table S8 Optimised atomic coordinates of heptanuclear cluster [**2**]$^{5+}$ obtained from DFT calculations

Number	Atom	x	y	z
1	Pt	2.271989	1.379703	1.518873
2	Pt	2.460830	–1.127635	–1.047146
3	Pt	5.147116	–0.102823	0.180290
4	Ag	–0.000559	0.156357	0.000575
5	S	3.215291	1.254608	–0.796718
6	S	3.072823	–0.987279	1.382286
7	N	0.563653	3.778165	2.172206
8	N	2.332082	4.501832	1.131429
9	N	0.457806	2.068613	3.828274
10	N	2.110897	0.897997	4.622954
11	N	1.124952	–1.900347	–3.633973
12	N	2.825913	–0.627461	–4.117466
13	N	1.018859	–3.607703	–1.964663
14	N	2.600115	–4.221156	–0.596340
15	N	7.515514	–0.328364	–1.619654
16	N	7.169456	1.796564	–1.285828
17	N	7.411592	–2.038813	0.041446
18	N	6.953803	–1.744118	2.151060
19	C	1.711455	3.343472	1.533756
20	C	0.482971	5.179742	2.187320
21	H	–0.320503	5.723147	2.657762
22	C	1.593219	5.631742	1.527080
23	H	1.923511	6.638680	1.327554
24	C	3.654372	4.607719	0.488282
25	H	3.808147	3.745724	–0.159077
26	H	4.439560	4.651462	1.250521
27	H	3.690386	5.523893	–0.107492
28	C	–0.329359	2.847693	2.868366
29	H	–0.810299	2.180378	2.148507
30	H	–1.097935	3.411858	3.400225

31	C	1.589786	1.372944	3.443212
32	C	0.289493	2.046029	5.221954
33	H	–0.515691	2.550155	5.731474
34	C	1.327253	1.304502	5.718215
35	H	1.580676	1.054913	6.736171
36	C	3.382720	0.169869	4.785780
37	H	4.218720	0.876828	4.804514
38	H	3.505077	–0.532815	3.962490
39	H	3.361603	–0.376058	5.732569
40	C	2.126163	–1.143808	–3.052502
41	C	1.203661	–1.862848	–5.035727
42	H	0.531731	–2.403347	–5.682818
43	C	2.267342	–1.055777	–5.336457
44	H	2.679089	–0.774668	–6.292809
45	C	4.046648	0.200009	–4.059074
46	H	4.787339	–0.204041	–4.755865
47	H	4.446483	0.184664	–3.046585
48	H	3.821428	1.234218	–4.337355
49	C	0.221668	–2.732426	–2.831396
50	H	–0.393561	–3.342531	–3.495983
51	H	–0.428998	–2.097353	–2.224106
52	C	2.003212	–3.105255	–1.133237
53	C	1.008169	–5.012159	–1.953706
54	H	0.335470	–5.606008	–2.551330
55	C	1.996154	–5.394202	–1.086649
56	H	2.328205	–6.379733	–0.800968
57	C	3.758905	–4.252072	0.317449
58	H	3.433152	–4.447783	1.343567
59	H	4.270106	–3.291041	0.286853
60	H	4.442583	–5.044842	–0.000197
61	C	6.668449	0.559088	–0.979223
62	C	8.529633	0.350651	–2.317328
63	H	9.302548	–0.149444	–2.879296
64	C	8.304018	1.685725	–2.113581
65	H	8.852894	2.544965	–2.465234
66	C	6.676976	3.082341	–0.765731
67	H	5.943835	2.880535	0.014532
68	H	6.219724	3.668513	–1.569646
69	H	7.511854	3.646710	–0.339467
70	C	7.408074	–1.776868	–1.403529
71	H	6.475695	–2.144445	–1.840384
72	H	8.254496	–2.282815	–1.871381
73	C	6.550646	–1.372332	0.895896
74	C	8.337044	–2.817203	0.758366
75	H	9.103906	–3.412518	0.288454
76	C	8.040834	–2.637538	2.083075
77	H	8.512761	–3.046479	2.962450
78	C	6.413134	–1.230843	3.419963
79	H	5.892892	–2.027505	3.961796

80	H	5.722958	–0.418457	3.195427
81	H	7.231887	–0.850485	4.038338
82	Pt	–2.274332	1.412316	–1.488334
83	Pt	–2.460049	–1.154755	1.017739
84	Pt	–5.145906	–0.098743	–0.184984
85	S	–3.215620	1.232987	0.826226
86	S	–3.074015	–0.958088	–1.407642
87	N	–0.562695	3.822710	–2.084705
88	N	–2.329044	4.524475	–1.025705
89	N	–0.462547	2.154341	–3.782609
90	N	–2.119139	1.007023	–4.604131
91	N	–1.122721	–1.991430	3.583840
92	N	–2.821028	–0.728051	4.099945
93	N	–1.018348	–3.656872	1.872542
94	N	–2.600126	–4.235236	0.489704
95	N	–7.500367	–0.358684	1.628571
96	N	–7.158483	1.772340	1.330615
97	N	–7.411866	–2.034412	–0.068353
98	N	–6.972080	–1.694467	–2.175047
99	C	–1.711241	3.374939	–1.456782
100	C	–0.477350	5.223890	–2.062667
101	H	0.327679	5.776798	–2.519166
102	C	–1.586411	5.661981	–1.391243
103	H	–1.914091	6.664429	–1.166321
104	C	–3.651879	4.617854	–0.382060
105	H	–3.818478	3.728366	0.223397
106	H	–4.433665	4.707381	–1.143782
107	H	–3.678244	5.505508	0.256024
108	C	0.327520	2.908370	–2.805236
109	H	0.809422	2.223005	–2.103116
110	H	1.095585	3.484783	–3.324597
111	C	–1.595500	1.451389	–3.413533
112	C	–0.296680	2.166748	–5.176764
113	H	0.509203	2.681350	–5.674609
114	C	–1.336487	1.439888	–5.689974
115	H	–1.591697	1.215923	–6.713466
116	C	–3.392591	0.286016	–4.785240
117	H	–3.544480	–0.392449	–3.947002
118	H	–3.348718	–0.287704	–5.714833
119	H	–4.221124	0.999355	–4.848671
120	C	–2.123257	–1.219344	3.021931
121	C	–1.199964	–1.988078	4.986192
122	H	–0.528288	–2.545249	5.619245
123	C	–2.262072	–1.186953	5.307586
124	H	–2.672353	–0.928462	6.270939
125	C	–4.040215	0.102763	4.062906
126	H	–4.782112	–0.318195	4.748328
127	H	–4.439211	0.115026	3.050073
128	H	–3.813211	1.128772	4.368742

129	C	–0.220410	–2.803712	2.760275
130	H	0.395251	–3.430323	3.408918
131	H	0.429893	–2.153816	2.168411
132	C	–2.002823	–3.133492	1.054337
133	C	–1.007222	–5.060592	1.825349
134	H	–0.334515	–5.669549	2.407540
135	C	–1.995715	–5.420375	0.949342
136	H	–2.327861	–6.398300	0.638766
137	C	–3.757649	–4.241649	–0.426385
138	H	–3.428268	–4.379807	–1.460565
139	H	–4.286553	–3.292704	–0.349271
140	H	–4.426907	–5.061174	–0.148826
141	C	–6.659168	0.541019	0.997666
142	C	–8.509218	0.306661	2.346696
143	H	–9.277584	–0.204313	2.905088
144	C	–8.286020	1.645425	2.165652
145	H	–8.832781	2.497588	2.537222
146	C	–6.668070	3.068006	0.833701
147	H	–5.975941	2.884004	0.012383
148	H	–6.163512	3.617622	1.635148
149	H	–7.512233	3.659818	0.467696
150	C	–7.395675	–1.802722	1.381530
151	H	–6.459605	–2.179396	1.802415
152	H	–8.238202	–2.318037	1.846154
153	C	–6.557485	–1.350777	–0.915740
154	C	–8.344336	–2.796222	–0.794059
155	H	–9.107750	–3.400903	–0.330524
156	C	–8.059367	–2.588199	–2.117158
157	H	–8.539732	–2.977022	–3.001090
158	C	–6.444461	–1.150426	–3.436724
159	H	–5.975732	–1.945060	–4.026276
160	H	–5.713005	–0.379201	–3.198213
161	H	–7.261605	–0.707872	–4.014744

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