Supplementary Information

Chloride assisted supramolecular assembly of a luminescent gigantic cluster: $[Ag_{216}S_{56}Cl_7(C{\equiv}CPh)_{98}(H_2O)_{12}]^{-}$ with pseudo-T_h skeleton and five-shell arrangement

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Additional Figures

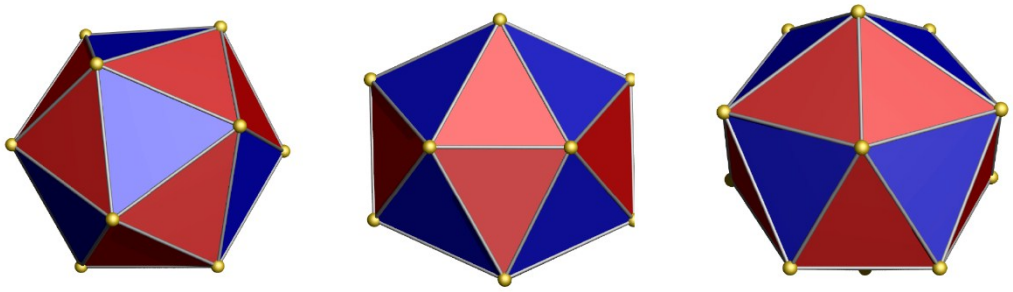

Fig. S1 The T_h-icosahedron in different view directions; The equilateral triangles are shown in blue and the isosceles triangles in red.

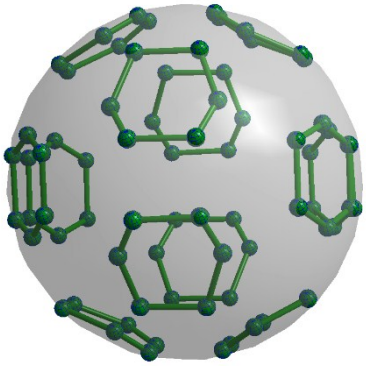

Fig. S2 Electron densities observed for shell-3, which are centered about 72 sites that form 12 six-membered rings arranged on a surface of a sphere of *ca*. 5.8 Å radius.

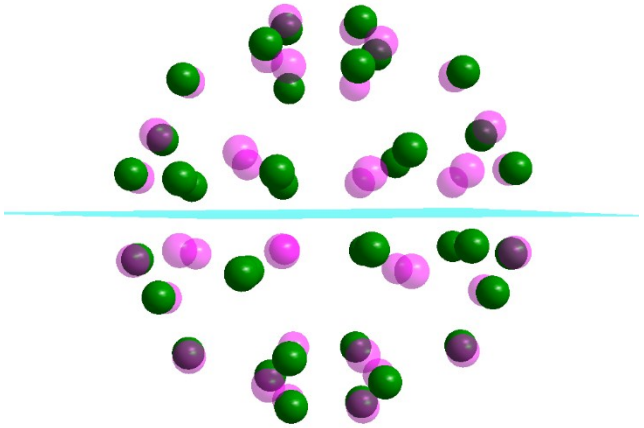

Fig. S3 The two disordered groups of silver atoms in shell-3 shown in green and pink respectively, which correspond to a reflection pair through the mirror plane.

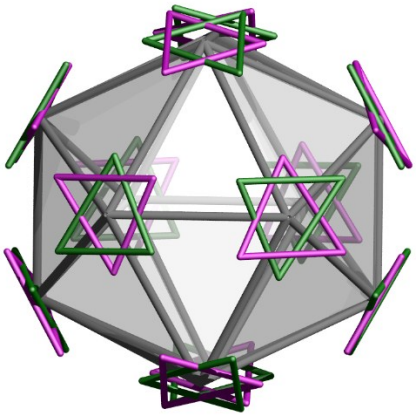

Fig. S4 The icosahedral arrangement of the 12 six-membered rings of Shell-3. The two disordered group of silver atoms are shown in green and pink respectively.

MALDI-MS spectrum

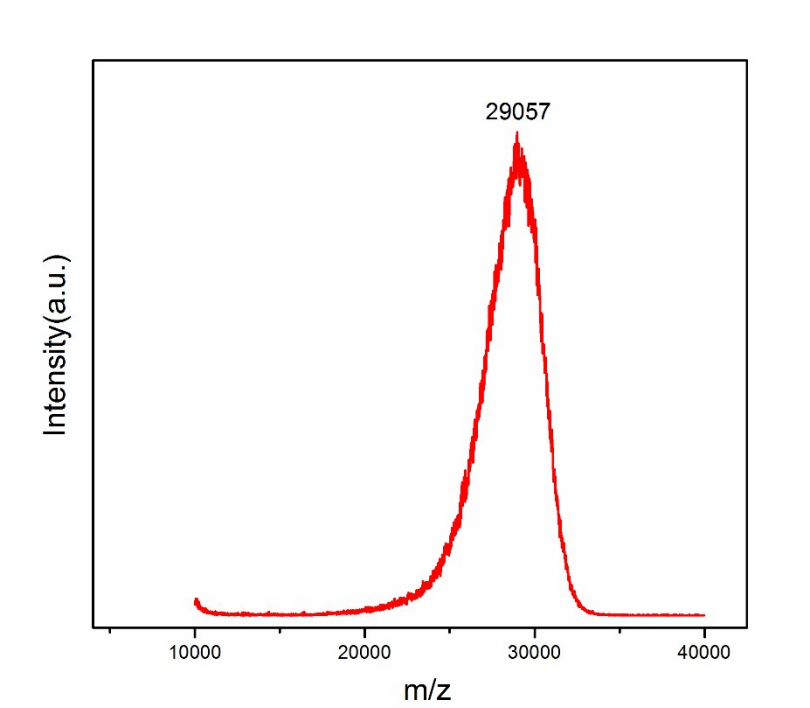

Fig. S5 The MALDI-MS spectrum of **1**.

NMR spectra

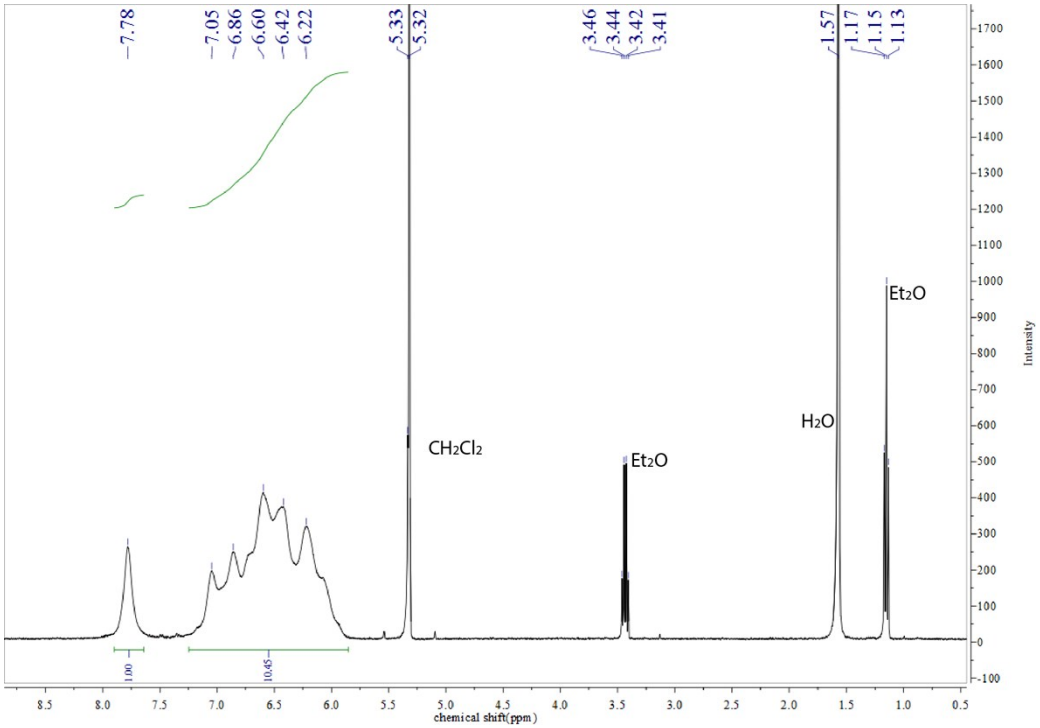

Fig. S6 ^{1}H NMR spectrum of compound **1** in CCl_2D_2.

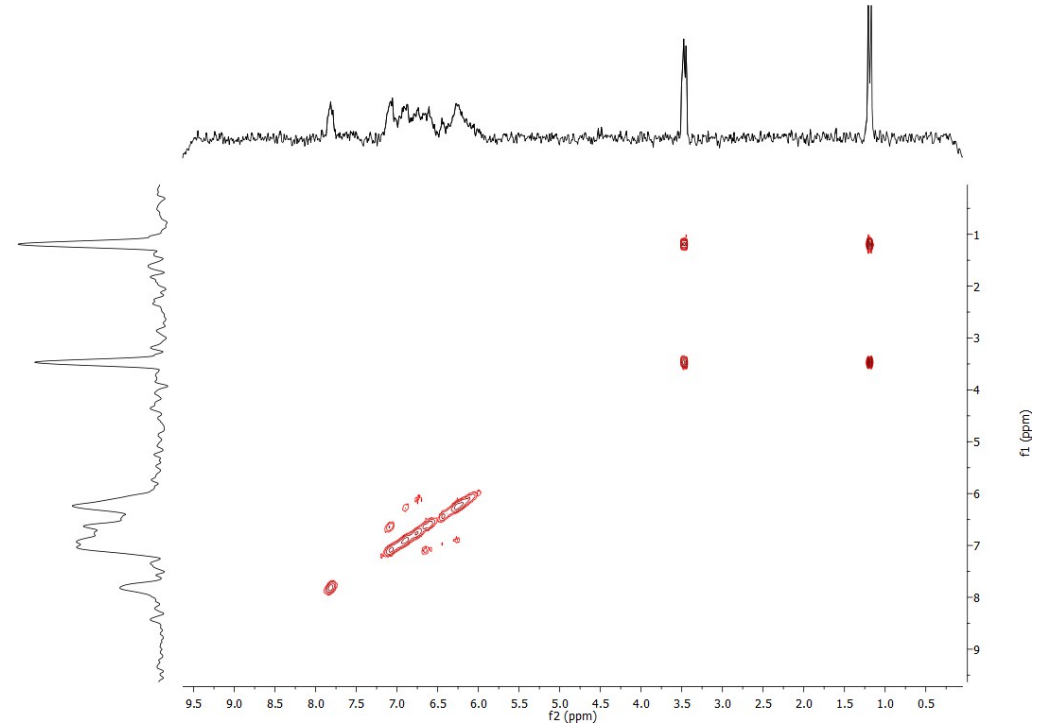

Fig. S7 2D ^{1}H NMR COSY spectrum of compound **1** in CCl_2D_2.

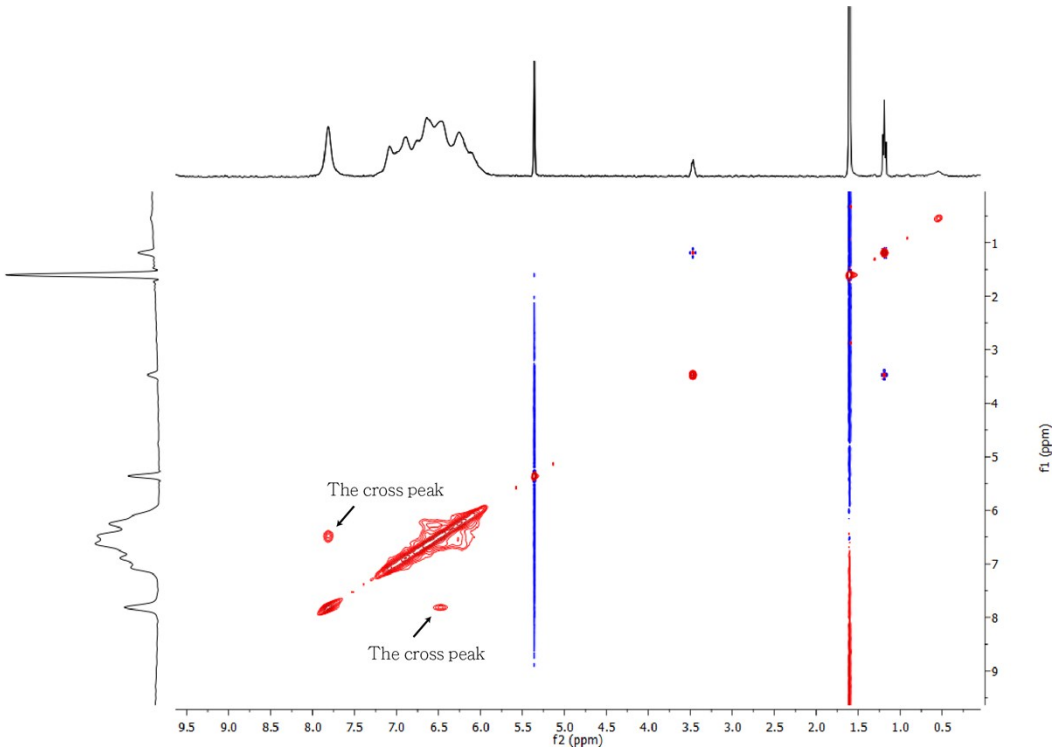

Fig. S8 2D ^{1}H NMR NOESY spectrum of compound **1** in CCl_2D_2.

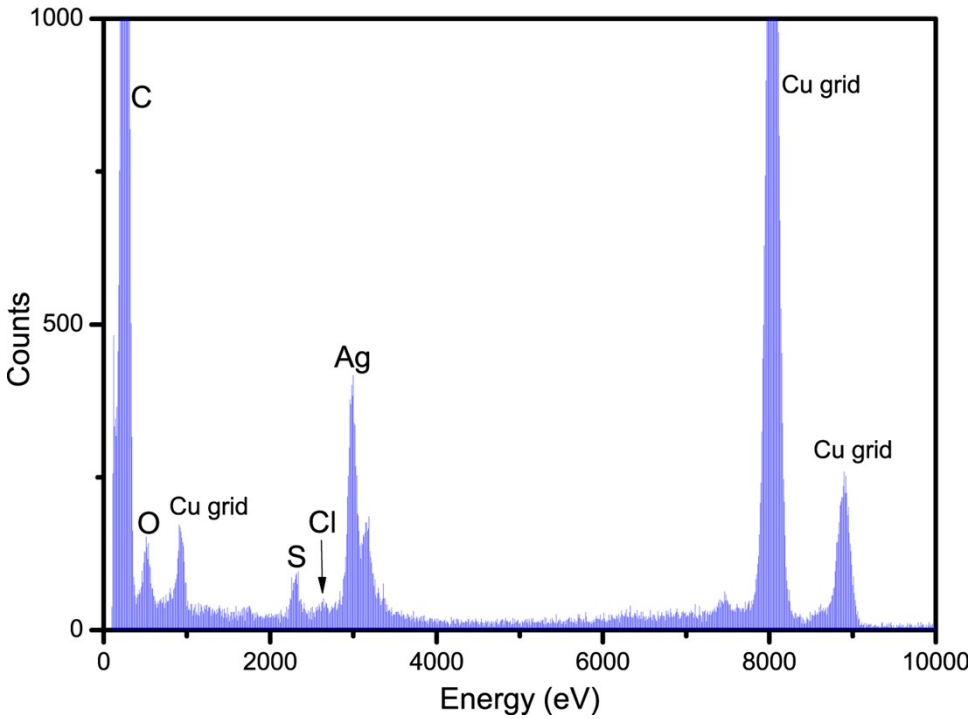

Fig. S9 EDX spectrum of compound **1**.

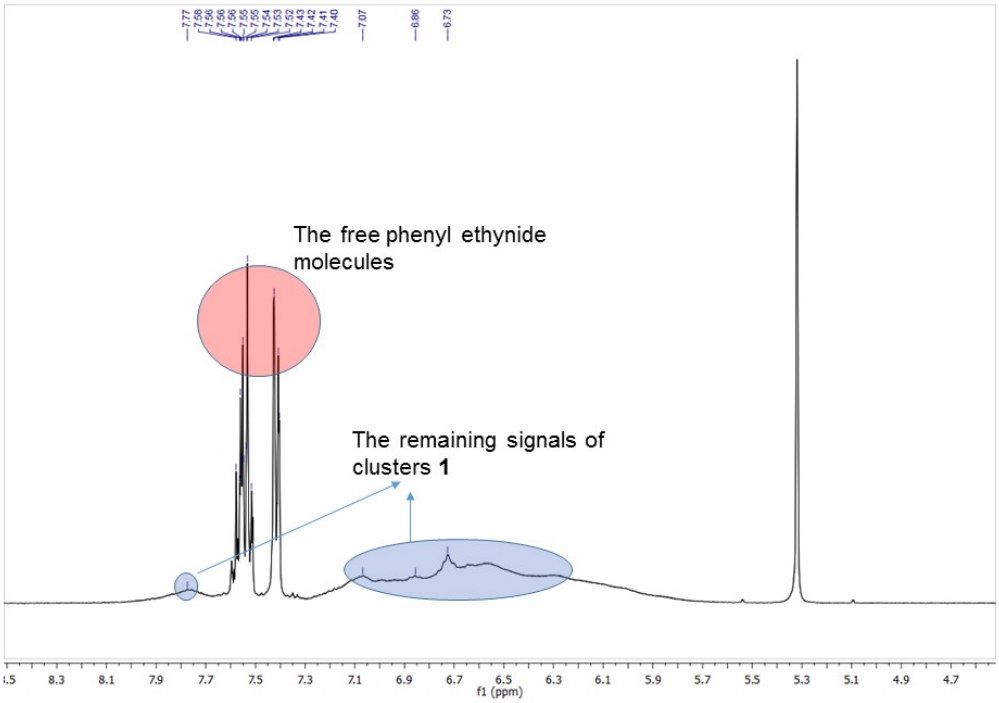

Fig. S10 ^{1}H NMR spectrum of compound **1** in CCl_2D_2 after heating under 40 ºC for 30 min.

The disordered silver sites and their occupancies

Ag4D	0.66(3)	Ag5N	0.34(3)
Ag35	0.51(2)	Ag3L	0.49(2)
Ag40	0.802(8)	Ag3K	0.198(8)
Ag4G	0.865(7)	Ag7L	0.135(7)
Ag7D	0.77(3)	Ag1O	0.23(3)
Ag5C	0.908(17)	Ag4	0.092(17)
Ag2D	0.660(7)	Ag5I	0.340(7)
Ag5E	0.767(14)	Ag5M	0.233(14)
Ag3F	0.639(6)	Ag6I	0.361(6)
Ag4C	0.57(3)	Ag4L	0.43(3)
Ag29	0.555(17)	Ag9K	0.445(17)
Ag37	0.833(6)	Ag7K	0.167(6)
Ag41	0.856(7)	Ag0N	0.144(7)
Ag6B	0.82(3)	Ag2P	0.18(3)
Ag3E	0.566(16)	Ag1L	0.434(16)
Ag2F	0.774(6)	Ag8J	0.226(6)
Ag1C	0.838(9)	Ag9J	0.162(9)
Ag0D	0.823(9)	Ag2K	0.177(9)
Ag2C	0.36(4)	Ag3P	0.64(4)
Ag6E	0.759(10)	Ag8I	0.241(10)
Ag24	0.62(3)	Ag2L	0.38(3)
Ag34	0.813(5)	Ag3I	0.187(5)
Ag42	0.744(8)	Ag9H	0.256(8)
Ag0C	0.837(7)	Ag2M	0.163(7)
Ag9B	0.853(10)	Ag6L	0.147(10)
Ag7C	0.830(7)	Ag9M	0.170(7)
Ag9C	0.61(5)	Ag4K	0.39(5)
Ag8B	0.762(7)	Ag9I	0.238(7)
Ag9E	0.750(7)	Ag8K	0.250(7)
Ag8C	0.633(8)	Ag18	0.367(8)
Ag2H	0.660(10)	Ag0R	0.340(10)
Ag0F	0.403(9)	Ag1M	0.597(9)
Ag4F	0.463(8)	Ag2I	0.537(8)
Ag8G	0.780(6)	Ag6J	0.220(6)
Ag1E	0.511(6)	Ag4I	0.489(6)
Ag1D	0.513(18)	Ag9L	0.487(18)
Ag0I	0.607(6)	Ag0K	0.393(6)
Ag1I	0.421(9)	Ag8O	0.579(9)

Ag0M	0.857(7)	Ag7N	0.143(7)		
Ag4H	0.524(14)	Ag6K	0.476(14)		
Ag8D	0.78(2)	Ag2N	0.22(2)		
Ag0H	0.887(7)	Ag1A	0.113(7)		
Ag7E	0.827(7)	Ag0Q	0.173(7)		
Ag8E	0.720(6)	Ag7I	0.280(6)		
Ag0P	0.520(11)	Ag9D	0.480(11)		
Ag5K	0.458(7)	Ag5L	0.542(7)		
Ag5	0.849(5)	Ag1F	0.151(5)		
Ag27	0.8	Ag5Q	0.1	Ag14	0.1
Ag6D	0.54(3)	Ag4M	0.46(3)		
Ag5G	0.36(5)	Ag8N	0.64(5)		
Ag8F	0.570(3)	Ag2J	0.354(3)	Ag0O	0.076(3)
Ag38	0.46(3)	Ag8L	0.54(3)		
Ag2E	0.477(3)	Ag7M	0.307(3)	Ag5O	0.216(3)
Ag0E	0.51	Ag4N	0.32	Ag7P	0.17
Ag5F	0.45	Ag1P	0.3	Ag6M	0.25