Electronic Supplementary Information

Understanding proton capture and cation-induced dimerization of $[Ag_{29}(BDT)_{12}]^{3-}$ clusters by ion mobility mass spectrometry

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Supplementary Information 1

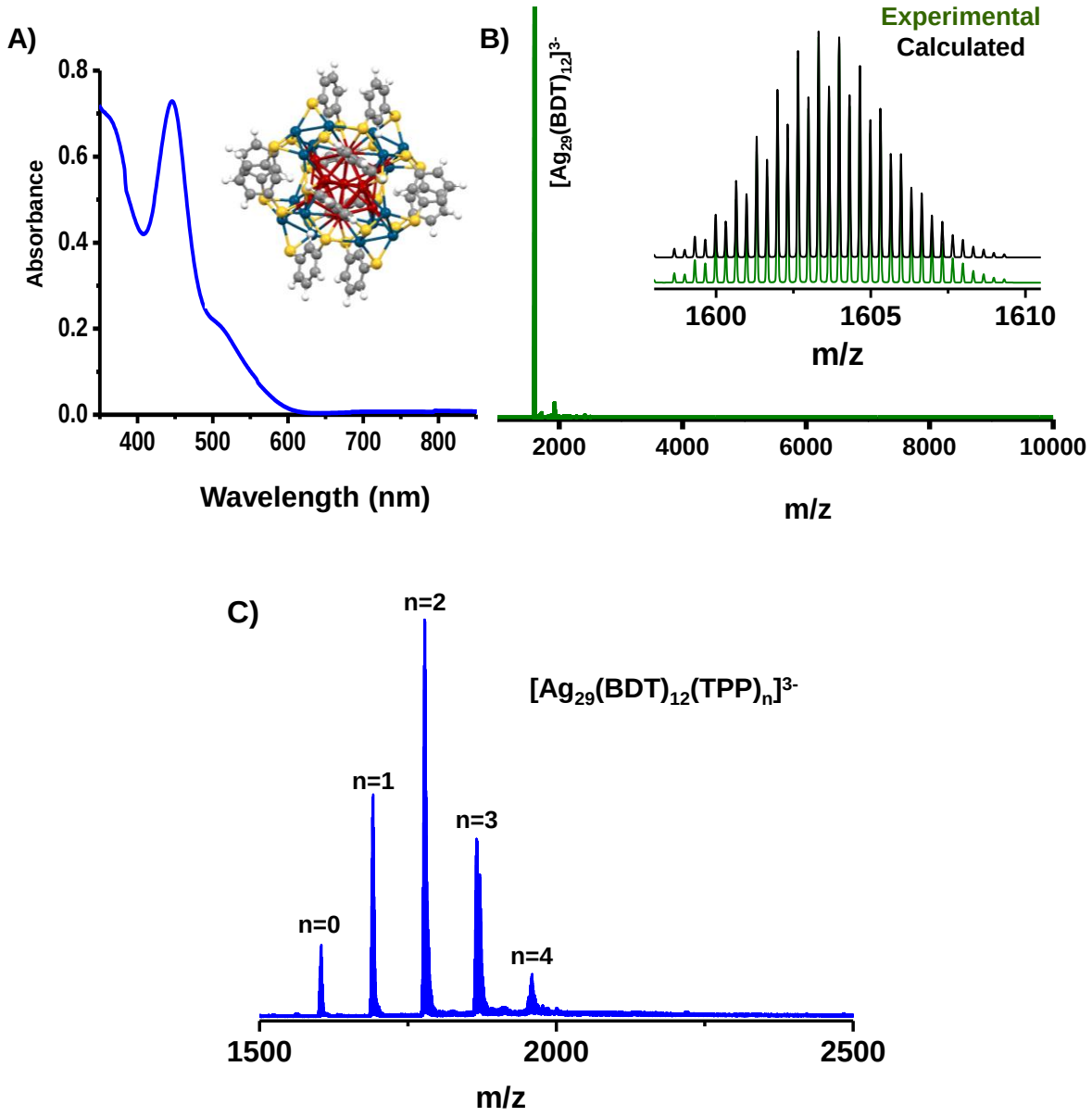

Fig. S1 A) UV-vis of $[Ag_{29}(BDT)_{12}(TPP)_4]^{3-}$ cluster, B) ESI MS of $[Ag_{29}(BDT)_{12}]^{3-}$, the TPP ligands are lost during the ionization. Inset of B) shows the experimental and calculated isotope patterns of $[Ag_{29}(BDT)_{12}]^{3-}$. The structure of $[Ag_{29}(BDT)_{12}]^{3-}$ is shown in the inset of A). C) ESI MS under the soft ionization conditions showing the intact $[Ag_{29}(BDT)_{12}(TPP)_n]^{3-}$ (n=1-4) clusters. Color codes: red: Ag atoms of the core; blue: Ag atoms of the staples; yellow: S; grey: C and white: H. The structure has been modelled taking the co-ordinates of its crystal structure.

Supplementary Information 2

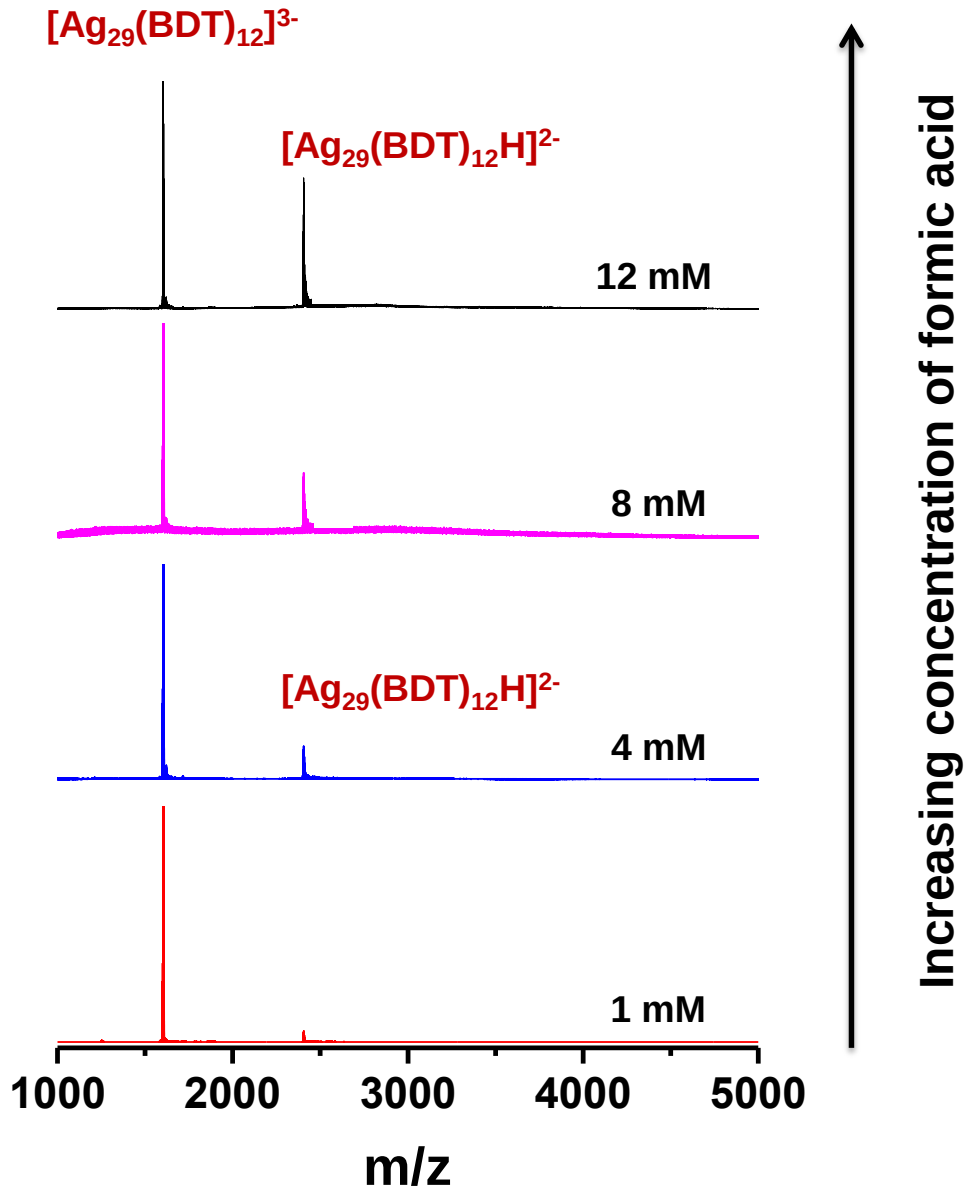

Fig. S2 ESI MS showing increase in the peak of $[Ag_{29}(BDT)_{12}H]^{2-}$ with increase in the concentration of formic acid. Formic acid concentration (mM) is indicated in the figure.

Supplementary Information 3

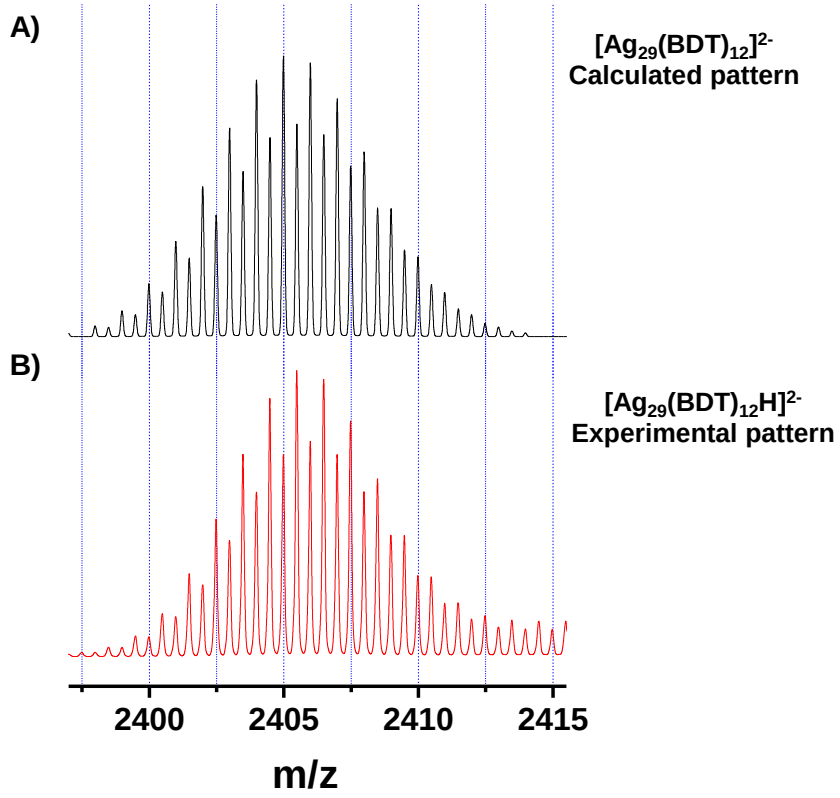

Fig. S3 A) Calculated isotope patterns of $[Ag_{29}(BDT)_{12}]^{2-}$ and B) experimental isotope pattern of $[Ag_{29}(BDT)_{12}H]^{2-}$. The isotope patterns show the difference between the two species. Experimental spectrum in the higher mass region overlaps with other features.

Supplementary Information 4

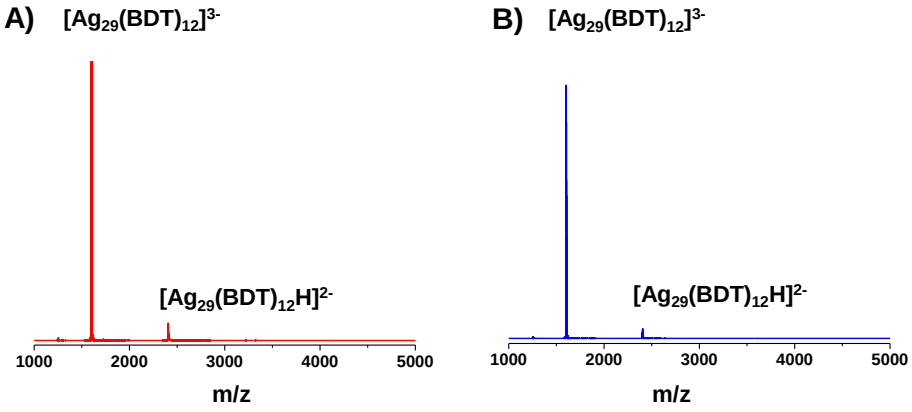

Fig. S4 ESI MS of $[Ag_{29}(BDT)_{12}]^{3-}$ in A) 1:1 DMF/MeOH mixture and B) DMF with one drop of H_2O added as the H^+ source. Peak for $[Ag_{29}(BDT)_{12}H]^{2-}$ was detected in both cases.

Supplementary Information 5

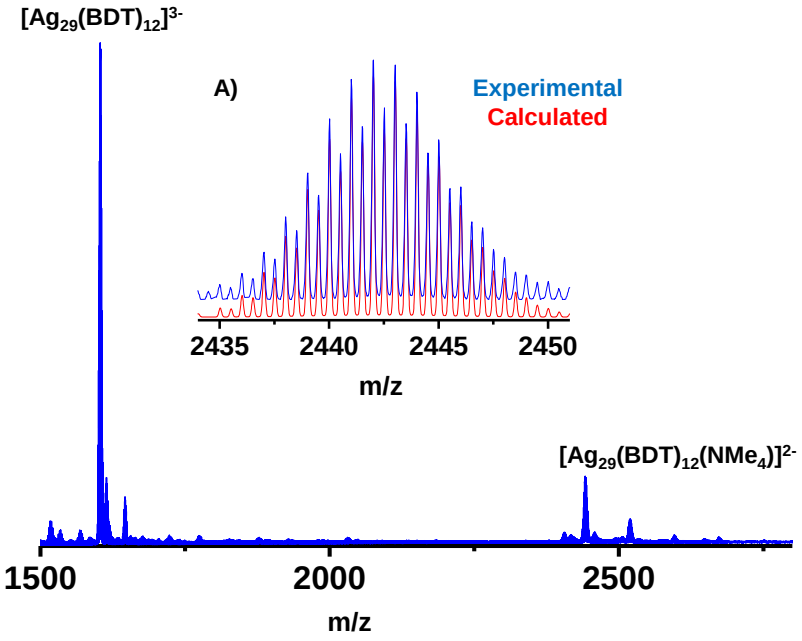

Fig. S5 ESI MS of $[Ag_{29}(BDT)_{12}]^{3-}$ cluster in presence of NMe_4Br. The cluster shows complexation with NMe_4^+ and hence a peak for the complex $[Ag_{29}(BDT)_{12}(NMe_4)]^{2-}$. Inset A) shows the comparison of experimental and calculated isotope patterns of $[Ag_{29}(BDT)_{12}(NMe_4)]^{2-}$.

Supplementary Information 6

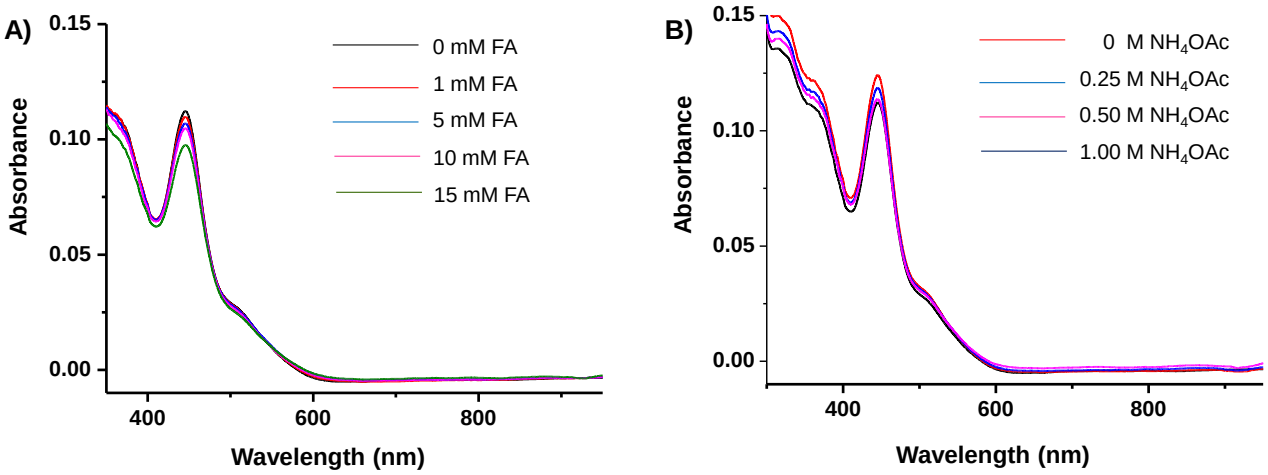

Fig. S6 UV-vis spectra of $[Ag_{29}(BDT)_{12}]^{3-}$ cluster in presence of different concentration of A) formic acid (FA) and B) NH_4OAc.

Supplementary Information 7

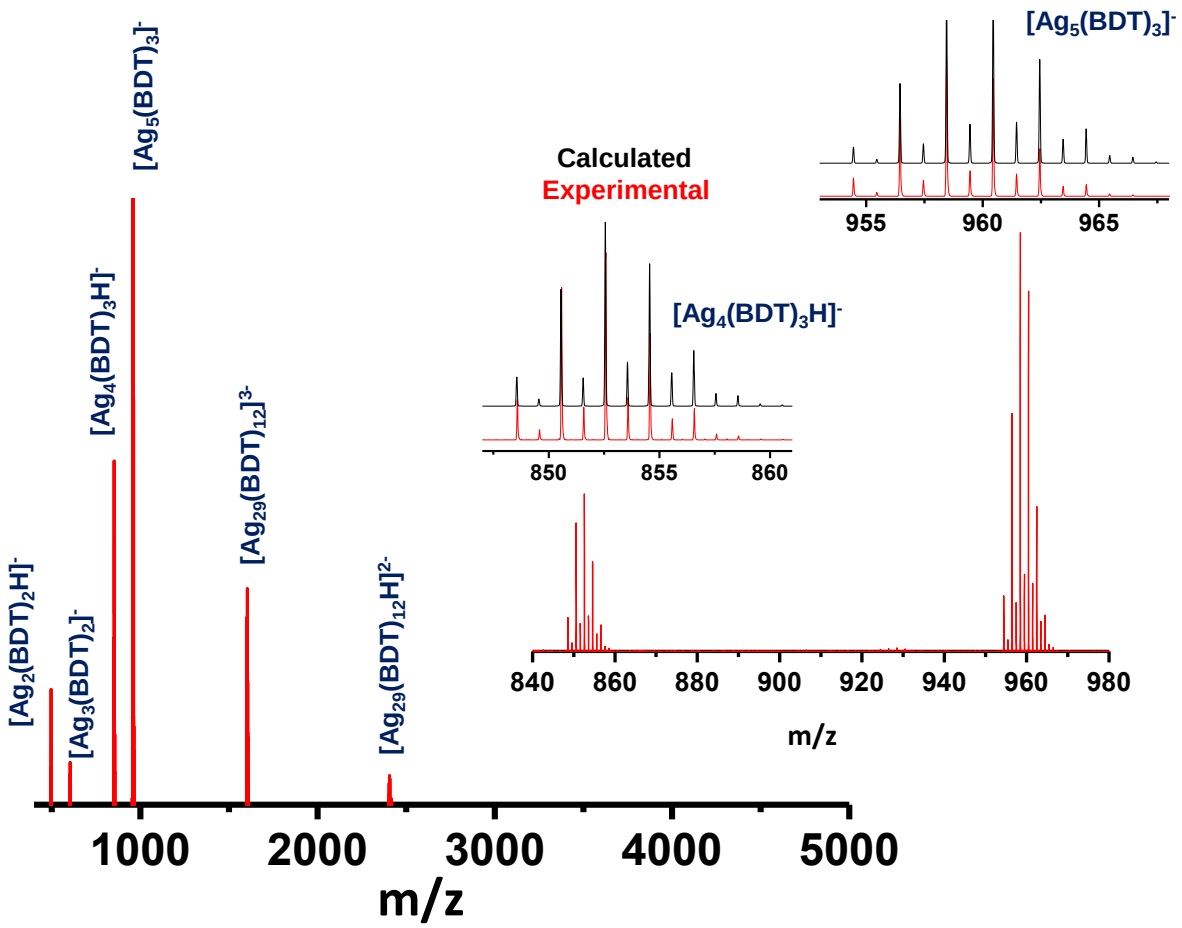

Fig. S7 MS/MS of $[Ag_{29}(BDT)_{12}H]^{2-}$. Inset shows the expanded view of the region from m/z 840 to 980 showing the fragments $[Ag_4(BDT)_3H]^-$ and $[Ag_5(BDT)_3]^-$. The theoretical and experimental isotope patterns of the fragments are also shown.

Supplementary Information 8

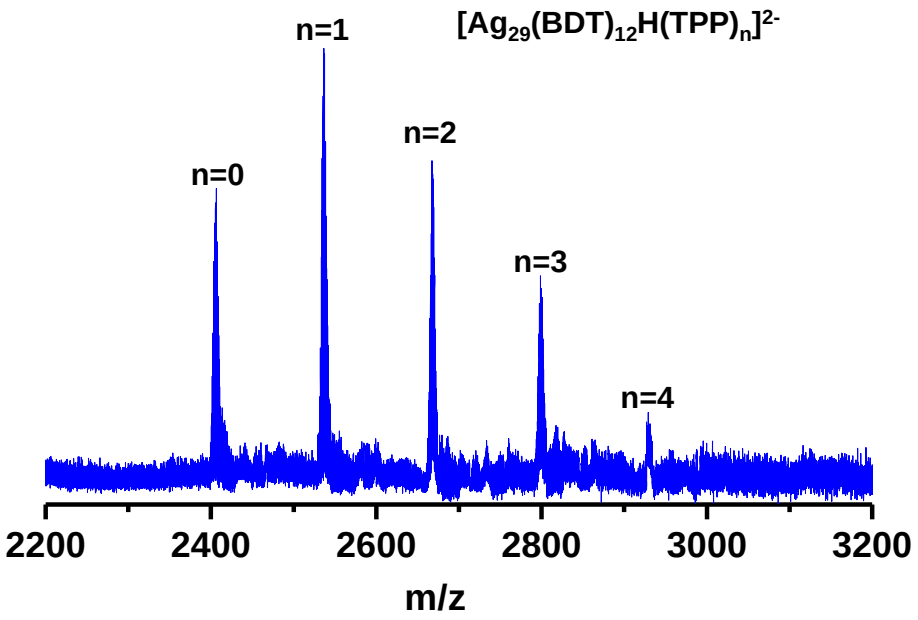

Fig. S8 ESI MS under soft ionization conditions showing the formation of intact $[Ag_{29}(BDT)_{12}H(TPP)_n]^{2-}$ (n=1-4) clusters.

Supplementary Information 9

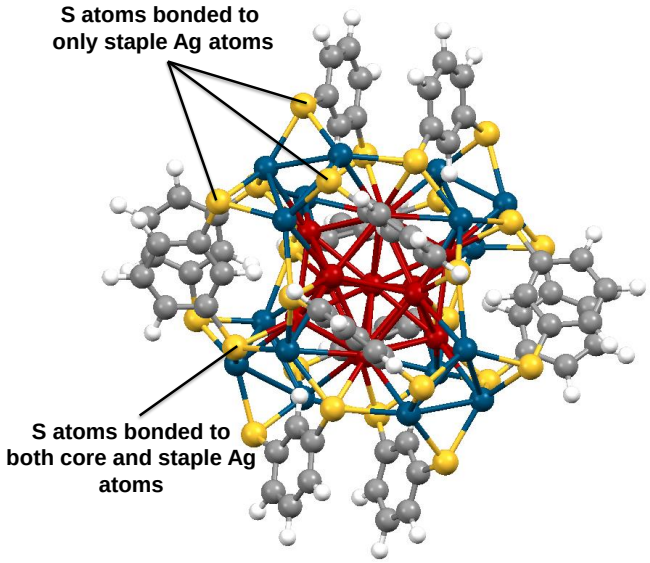

Fig. S9 Structure of $[Ag_{29}(BDT)_{12}]^{3-}$ cluster showing two different types of S atoms in the exterior shell. Color codes: red: Ag atoms of the core; blue: Ag atoms of the staples; yellow: S; grey: C and white: H.

Supplementary Information 10

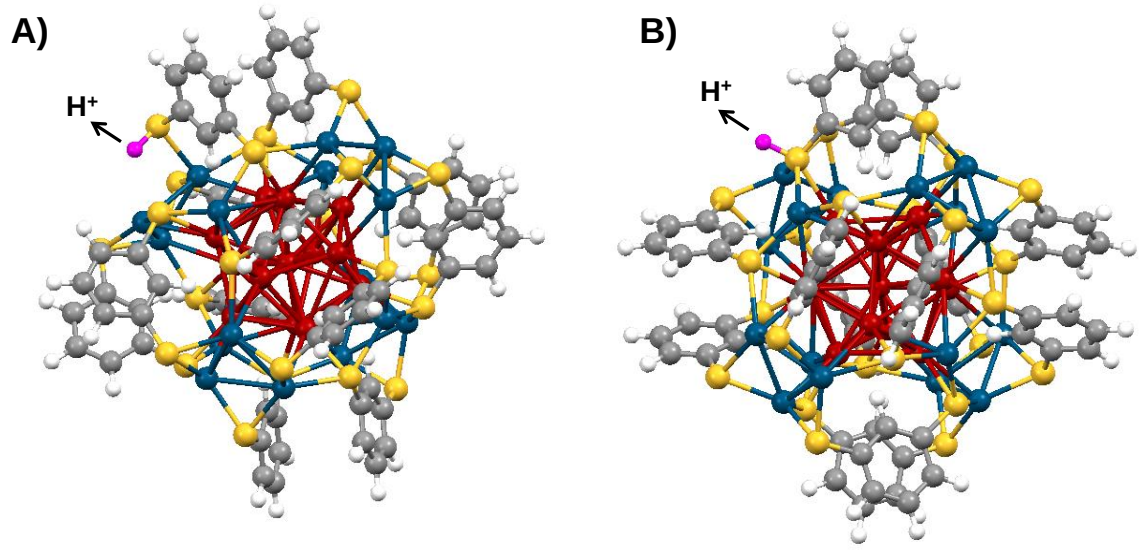

Fig. S10 Structure of $[Ag_{29}(BDT)_{12}H]^{2-}$ with proton attached to S atom A) bonded to only Ag atoms of the staples and B) bonded to both staple and core Ag atoms. Color codes: red: Ag atoms of the core; blue: Ag atoms of the staples; yellow: S; grey: C, white: H and purple: proton.

Supplementary Information 11

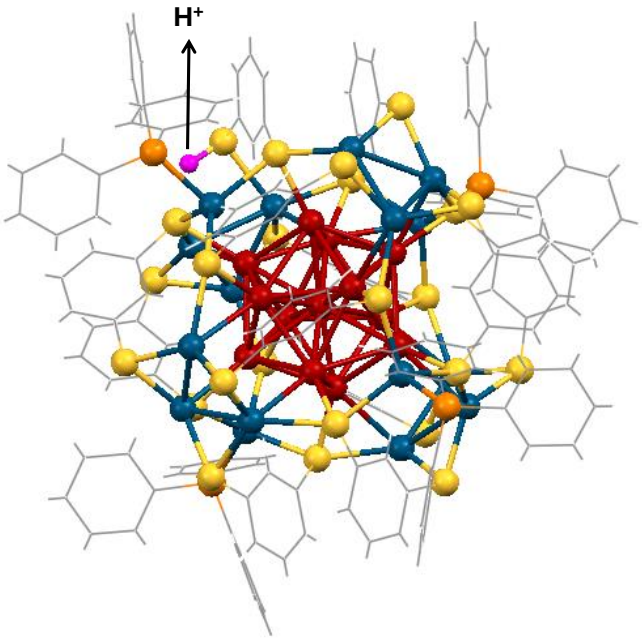

Fig. S11 Structure of $[Ag_{29}(BDT)_{12}H(TPP)_4]^{2-}$. S-H bond distance is 1.38 Å and binding energy of proton is -73.92 kcal/mol. The P atoms are shown in orange color and thickness of the bonds in the ligands has been reduced for better clarity, proton is shown in purple color.

Supplementary Information 12

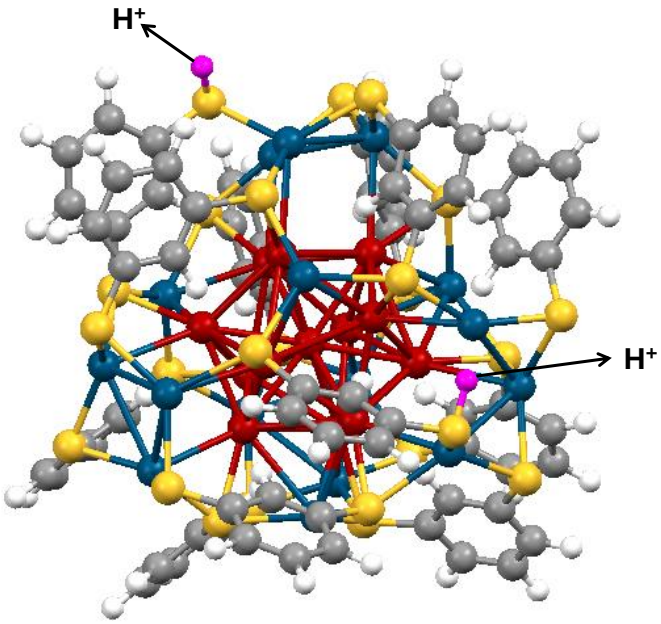

Fig. S12 DFT optimized structure of $[Ag_{29}(BDT)_{12}H_2]^{-}$. Proton is shown in purple color.

Supplementary Information 13

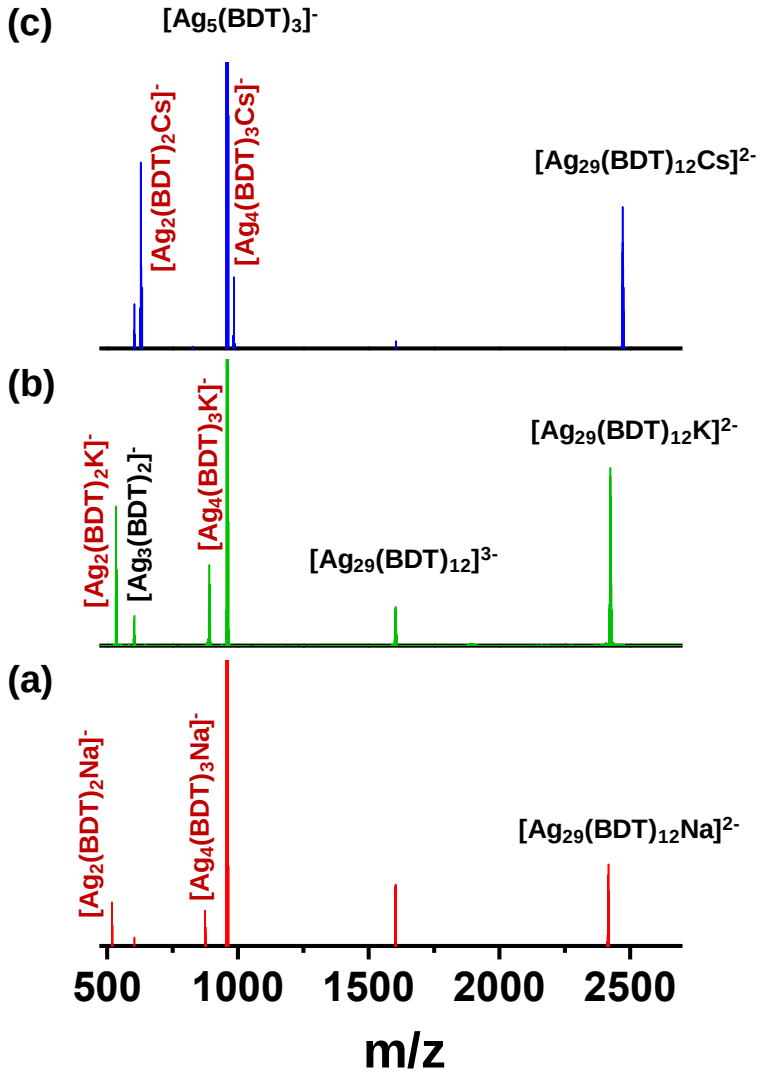

Fig. S13 MS/MS of (a) $[Ag_{29}(BDT)_{12}Na]^{2-}$, (b) $[Ag_{29}(BDT)_{12}K]^{2-}$ and (c) $[Ag_{29}(BDT)_{12}Cs]^{2-}$.

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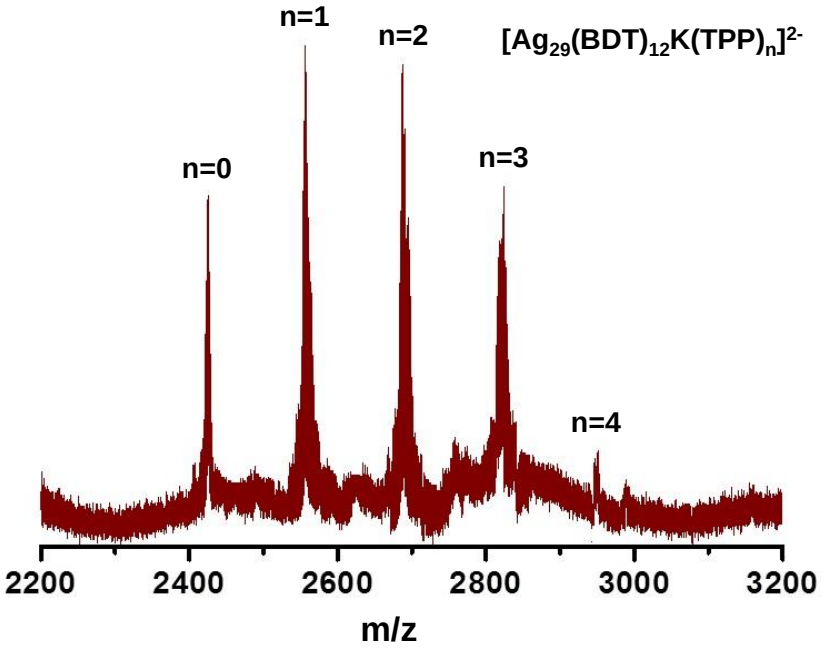

Fig. S14. ESI MS under soft ionization conditions showing the formation of intact $[Ag_{29}(BDT)_{12}K(TPP)_n]^{2-}$ (n=1-4) clusters.

Supplementary Information 15

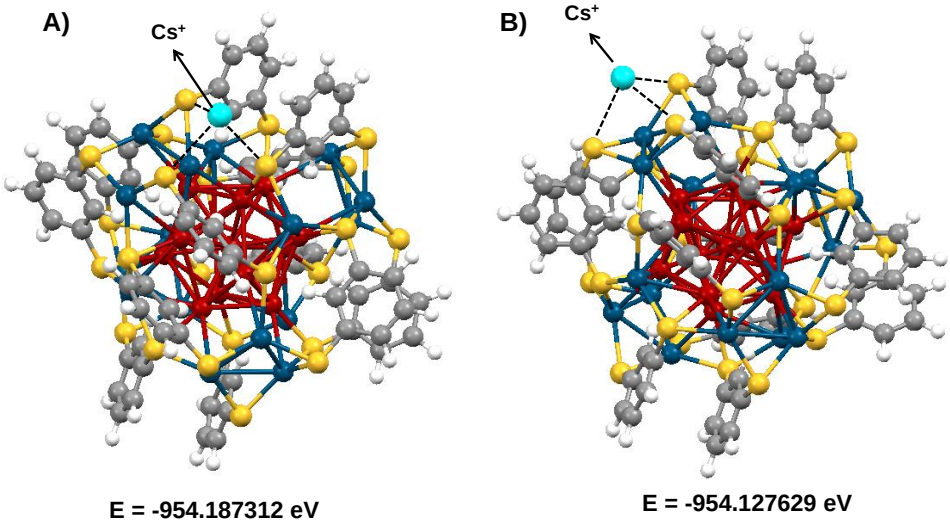

Fig. S15 DFT optimized structure of $[Ag_{29}(BDT)_{12}Cs]^{2-}$ with A) Cs^+ attached to S atoms one of which is attached to a core Ag atom and B) all S atoms are attached only to staple Ag atoms. Relative energies of A) 0 kcal/mol and B) 1.38 kcal/mol.

Supplementary Information 16

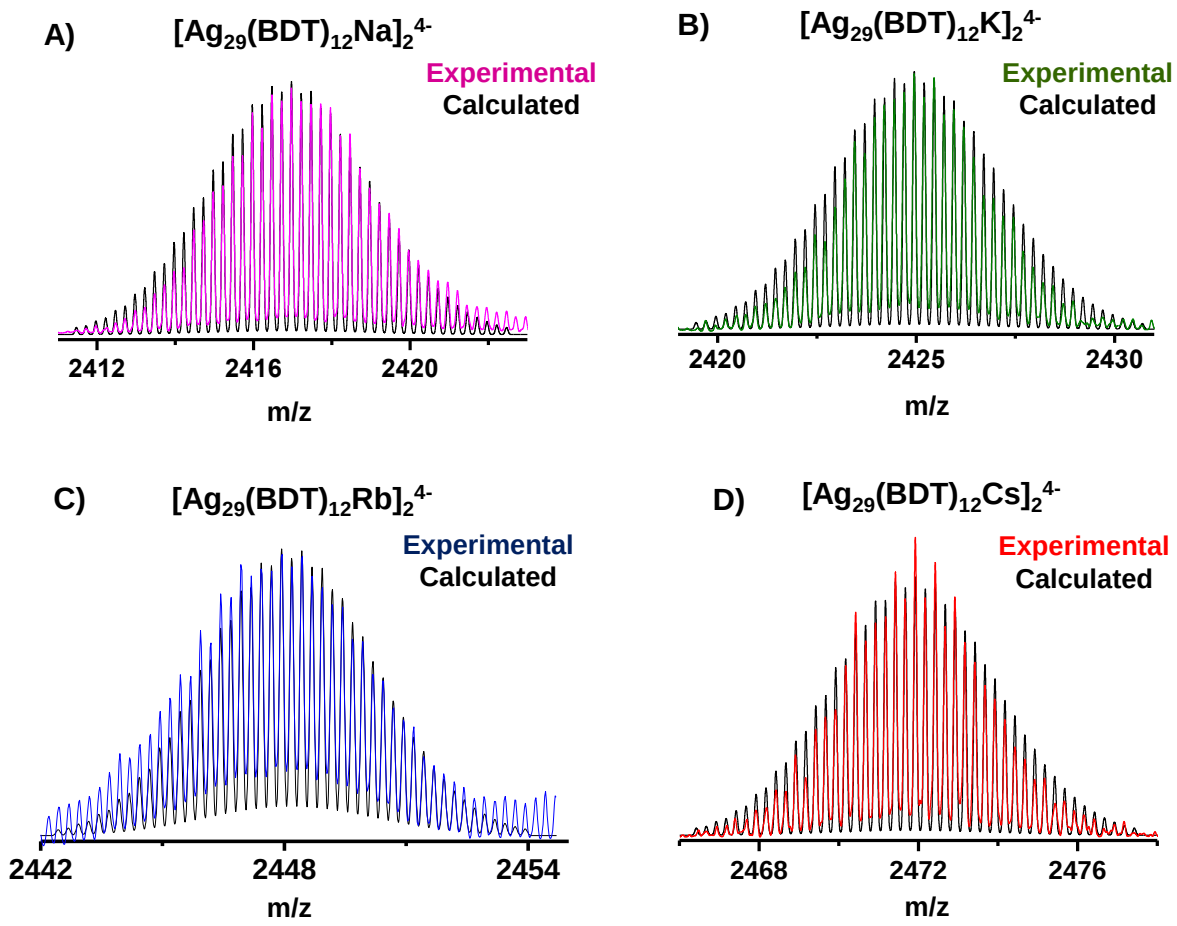

Fig. S16 Experimental and calculated isotope patterns of the dimers A) $[Ag_{29}(BDT)_{12}Na]_2^{4-}$, B) $[Ag_{29}(BDT)_{12}K]_2^{4-}$, C) $[Ag_{29}(BDT)_{12}Rb]_2^{4-}$ and D) $[Ag_{29}(BDT)_{12}Cs]_2^{4-}$.

Supplementary Information 17

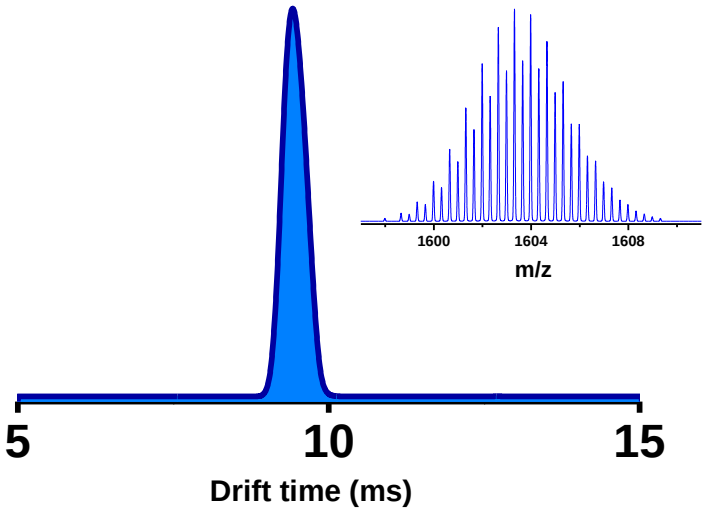

Fig. S17 Drift time profile of $[Ag_{29}(BDT)_{12}]^{3-}$ showing only a single peak for the monomer. Inset shows the ESI MS corresponding to the mobilogram.

Supplementary Information 18

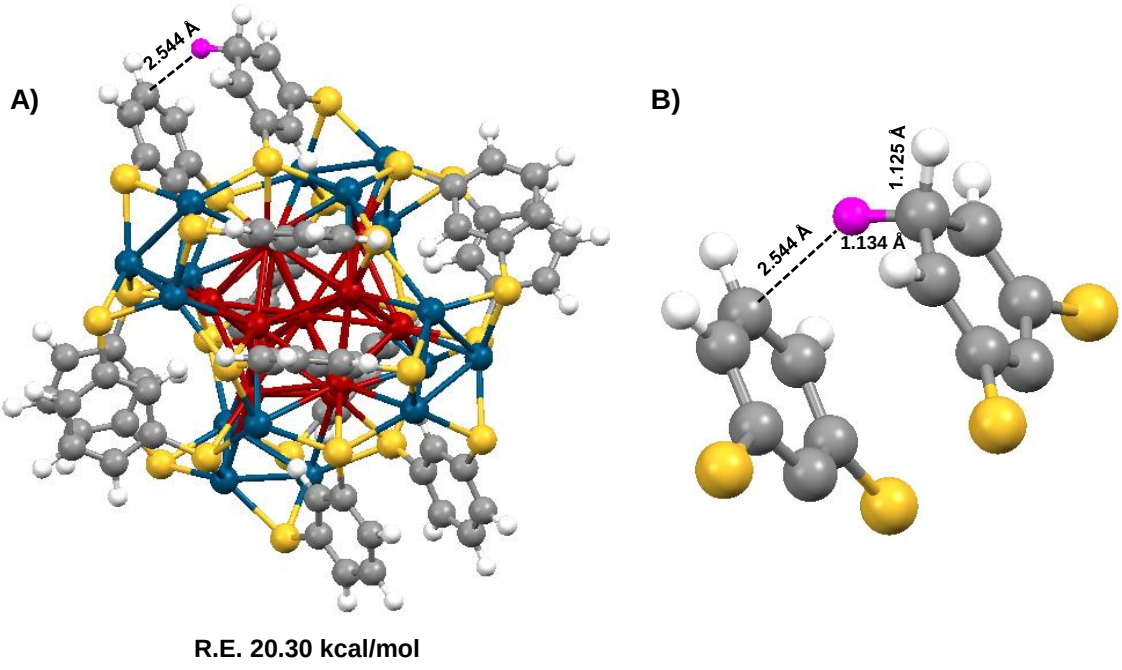

Fig. S18 A) DFT optimized structure of $[Ag_{29}(BDT)_{12}H]^{2-}$ with proton sandwiched between the two benzene rings of the BDT ligands. B) Expanded view showing the conformation of the proton sandwiched between the two benzene rings. Proton is colored in purple.

Supplementary Information 19

Species (Monomers)	CCS values (Å²)
$[Ag_{29}(BDT)_{12}H]^{2-}$	535.57
$[Ag_{29}(BDT)_{12}Li]^{2-}$	535.92
$[Ag_{29}(BDT)_{12}Na]^{2-}$	537.52
$[Ag_{29}(BDT)_{12}K]^{2-}$	539.78
$[Ag_{29}(BDT)_{12}Rb]^{2-}$	543.67
$[Ag_{29}(BDT)_{12}Cs]^{2-}$	547.92

Species (Dimers)	CCS values (Å²)
$[Ag_{29}(BDT)_{12}Na]_2^{4-}$	877.31
$[Ag_{29}(BDT)_{12}K]_2^{4-}$	880.51
$[Ag_{29}(BDT)_{12}Rb]_2^{4-}$	887.30
$[Ag_{29}(BDT)_{12}Cs]_2^{4-}$	894.72

Fig. S19 CCS values of the monomers $[Ag_{29}(BDT)_{12}M]^{2-}$ (M=H, Li, Na, K, Rb, Cs) and the dimers $[Ag_{29}(BDT)_{12}M]_2^{4-}$ (M=Na, K, Rb, Cs) measured from IM MS.

Supplementary Information 20

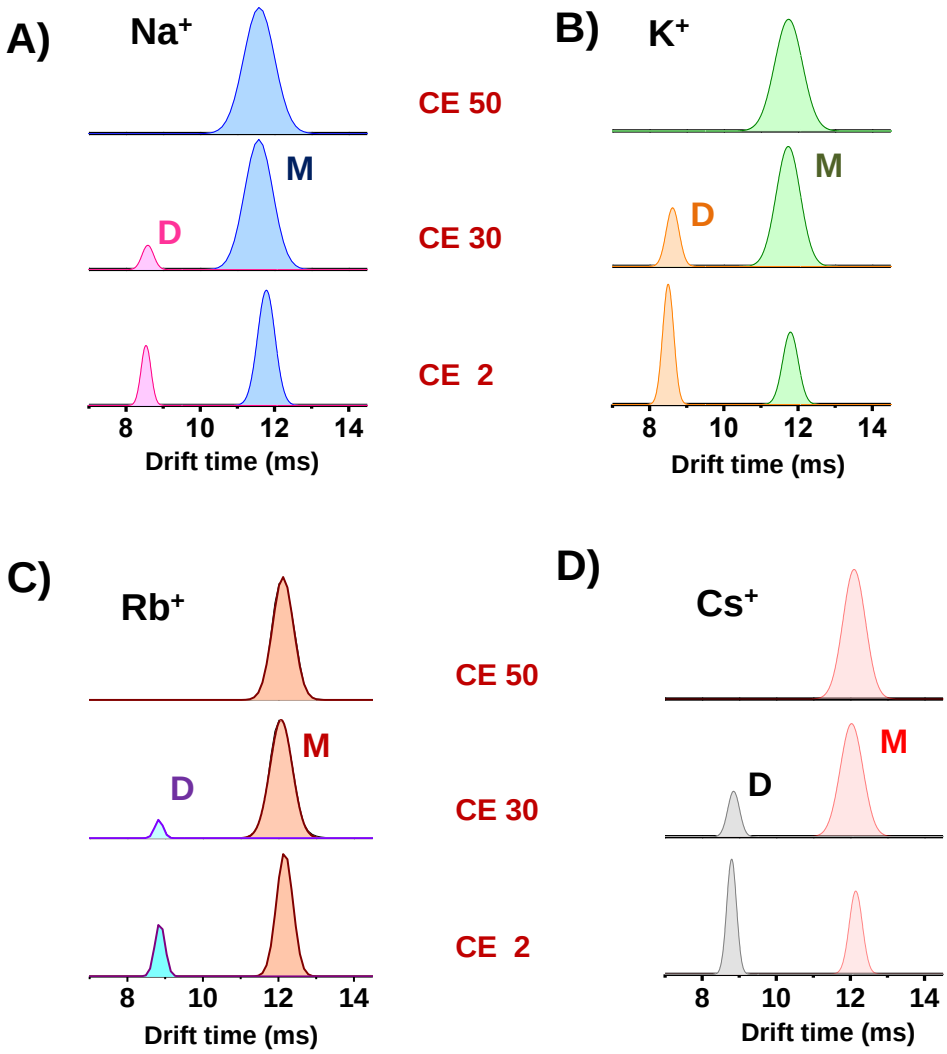

Fig. S20 CID of the dimers $[Ag_{29}(BDT)_{12}M]_2^{4-}$, A) M=Na, B) M=K, C) M=Rb and D) M=Cs.

Supplementary Information 21

Cartesian coordinates of the DFT optimized lowest energy structures

1. Lowest energy structure of $[Ag_{29}(BDT)_{12}H]^{2-}$

Ag	12.12766	11.84008	12.01999
Ag	14.14016	13.63322	10.95673
Ag	12.34732	14.27013	13.43560
Ag	11.08233	14.08635	10.69810
Ag	10.29240	9.92083	13.11112
Ag	17.18262	14.32407	10.82974
Ag	12.93858	16.30210	11.36363
Ag	11.06812	15.86380	15.53885
Ag	9.23988	15.12299	8.71579
Ag	8.46109	14.53151	15.48484
Ag	7.63643	11.04486	12.40879
S	16.08939	12.30479	15.49843
S	12.86353	16.76545	13.83854
S	10.78274	16.58668	9.95942
S	8.02919	9.03544	13.88296
S	18.15181	15.16647	12.97794
S	12.14824	15.40121	17.87582
S	8.85050	16.97962	15.22178
S	8.08747	13.24027	17.61022
C	15.59368	13.69200	16.50911
C	16.59040	14.38601	17.23824
H	17.65286	14.11403	17.09193
C	16.23151	15.40103	18.14352
H	17.02116	15.93002	18.71159
C	14.88287	15.73914	18.35886
H	14.60110	16.50926	19.10220
C	13.89528	15.07864	17.59741
C	14.24078	14.07569	16.67305
H	13.45302	13.58586	16.06329
C	14.60781	16.82307	14.25914
C	15.05527	17.83715	15.13709
H	14.32178	18.50916	15.62184
C	16.43800	17.99457	15.35534
H	16.79341	18.79078	16.03909
C	17.37381	17.17243	14.70391
H	18.45943	17.32342	14.85896
C	16.93277	16.14298	13.83048

C	15.54432	15.97269	13.63630
H	15.19288	15.16526	12.96043
C	9.60929	17.24053	11.16748
C	9.61463	16.79520	12.50615
H	10.27577	15.95500	12.80378
C	8.80624	17.41264	13.48813
C	7.95702	18.47721	13.09175
H	7.32747	18.97959	13.85091
C	7.92363	18.89241	11.74888
H	7.24797	19.71813	11.45076
C	8.74629	18.28882	10.77824
H	8.73373	18.63482	9.72757
C	7.65321	9.69823	15.50851
C	8.05005	10.99559	15.89582
H	8.72055	11.57489	15.22790
C	7.60650	11.57920	17.10436
C	6.75990	10.82524	17.95246
H	6.40093	11.26733	18.90178
C	6.38983	9.51734	17.58495
H	5.73328	8.93146	18.25821
C	6.82904	8.94286	16.37730
H	6.52651	7.91752	16.09219
Ag	14.57966	10.82296	11.01006
Ag	12.35392	12.03352	9.21788
Ag	11.78429	9.34962	10.72547
Ag	9.76635	13.01636	13.14855
Ag	17.56469	11.34773	10.57893
Ag	13.73919	9.55782	8.43322
Ag	10.88793	12.88166	6.76239
Ag	11.49647	6.34311	11.05050
Ag	8.09106	12.50804	7.97804
S	15.04959	15.86772	10.07581
S	13.17304	11.53739	6.87287
S	12.01254	7.74500	8.78677
S	7.22775	13.27529	13.55354
S	18.14799	13.12352	8.87991
S	11.39748	15.27926	5.85530
S	8.99678	11.49258	5.90386
S	6.89583	14.73342	8.16886
C	14.57902	16.02442	8.36027
C	15.45195	16.73082	7.49463
H	16.42739	17.08079	7.88379
C	15.07452	16.99663	6.16792
H	15.76233	17.55691	5.50612

C	13.82417	16.57575	5.67567
H	13.50721	16.81392	4.64354
C	12.97052	15.84497	6.52873
C	13.34886	15.54751	7.85119
H	12.67711	14.94316	8.49571
C	14.73133	12.40773	6.69305
C	15.09855	12.87808	5.41045
H	14.39502	12.77364	4.56244
C	16.37333	13.44858	5.22782
H	16.66655	13.81401	4.22390
C	17.28707	13.54368	6.29228
H	18.29365	13.97690	6.13577
C	16.92864	13.07249	7.58250
C	15.63995	12.52403	7.76474
H	15.35489	12.14634	8.76789
C	10.66735	8.15279	7.67189
C	10.33329	9.48971	7.36901
H	10.83763	10.31385	7.91409
C	9.38332	9.80701	6.37432
C	8.73953	8.74595	5.68867
H	7.99050	8.97370	4.90623
C	9.04627	7.41208	6.01529
H	8.52816	6.58827	5.48531
C	10.00392	7.10134	6.99885
H	10.24810	6.05179	7.24776
C	6.60158	14.35376	12.27004
C	6.99367	14.18743	10.92670
H	7.78341	13.44908	10.68059
C	6.39916	14.93337	9.88537
C	5.37908	15.86087	10.20973
H	4.89588	16.44781	9.40566
C	4.99605	16.03745	11.55319
H	4.19917	16.76670	11.80071
C	5.60119	15.30236	12.59019
H	5.29047	15.44558	13.64270
Ag	14.56979	12.31734	13.43863
Ag	13.11700	9.47201	13.24184
Ag	11.82524	11.81259	14.79417
Ag	9.78658	11.54266	10.40601
Ag	17.62538	12.73191	13.28901
Ag	14.29516	10.53575	15.79093
Ag	12.60453	6.52623	13.87518
Ag	10.43216	12.80926	17.13157
Ag	9.67755	6.90629	13.40637

S	16.04943	9.45337	9.47365
S	14.47761	8.17858	14.95007
S	12.30053	11.21372	17.29607
S	7.38451	10.85042	9.90927
S	18.89358	10.69739	12.59865
S	13.48891	5.15473	11.98646
S	10.75661	6.13345	15.52712
S	9.09064	5.70884	11.29863
C	16.09814	7.84543	10.27090
C	17.30764	7.11391	10.24960
H	18.22149	7.56964	9.82335
C	17.32703	5.80790	10.77653
H	18.27352	5.23247	10.76304
C	16.16864	5.22016	11.31443
H	16.19369	4.19029	11.71931
C	14.95243	5.95078	11.34997
C	14.94166	7.26386	10.83083
H	13.99323	7.83943	10.85647
C	16.15266	8.13582	14.30568
C	16.93547	6.98566	14.55504
H	16.47874	6.10569	15.04547
C	18.29481	6.98979	14.18767
H	18.91359	6.09185	14.38543
C	18.88372	8.11666	13.58741
H	19.95706	8.11591	13.31825
C	18.10124	9.26924	13.31756
C	16.73459	9.25170	13.67044
H	16.11713	10.14843	13.45400
C	11.32663	9.70691	17.49570
C	11.35053	8.69952	16.51074
H	11.90863	8.86542	15.56740
C	10.67758	7.47036	16.70072
C	9.95172	7.28277	17.90651
H	9.41343	6.32908	18.06885
C	9.91206	8.29810	18.87898
H	9.33453	8.13899	19.81164
C	10.59906	9.51287	18.69179
H	10.57252	10.30543	19.46323
C	7.41812	9.07941	9.61850
C	8.23874	8.22607	10.38330
H	8.96486	8.66164	11.10065
C	8.13085	6.82102	10.28752
C	7.18732	6.27594	9.37829
H	7.08354	5.17650	9.29813

C	6.39246	7.12809	8.59074
H	5.66289	6.69089	7.88024
C	6.49560	8.52847	8.69983
H	5.85629	9.19818	8.09399
H	10.57455	15.96614	6.73137
H	12.27233	16.73926	18.16195

2. Lowest energy structure of $[Ag_{29}(BDT)_{12}Na]^{2-}$

Ag	11.95973	12.00974	11.99381
Ag	14.42864	12.16314	13.48003
Ag	13.40786	14.49236	12.14506
Ag	12.09081	13.43340	14.44515
Ag	11.94554	10.45090	14.36655
Ag	14.33432	12.18867	10.56967
Ag	10.41898	14.38335	11.91192
Ag	13.55040	9.62893	11.78774
Ag	11.77999	13.55548	9.57835
Ag	9.57844	11.78097	13.48966
Ag	9.52745	12.06769	10.49916
Ag	10.57998	9.52315	12.05734
Ag	12.10206	10.58496	9.50575
Ag	16.19958	13.77189	15.35536
Ag	15.37121	16.20265	13.78583
Ag	13.74582	15.34684	16.16968
Ag	14.69966	9.38179	14.54317
Ag	14.49618	14.81571	9.29519
Ag	9.34341	14.52767	14.68794
Ag	10.32328	8.49118	16.10779
Ag	14.94163	9.90605	9.16855
Ag	8.48787	16.10670	10.28548
Ag	15.32934	7.35410	10.26613
Ag	10.07172	15.38439	7.82215
Ag	7.85206	10.07064	15.37251
Ag	8.65487	7.70567	13.72820
Ag	13.49063	8.30243	7.38777
Ag	7.72666	13.71498	8.60723
Ag	9.35375	9.33302	9.35394
S	11.16450	14.67550	16.45022
S	16.48411	11.17366	14.63075
S	14.66867	16.47795	11.17308
S	12.91604	9.14432	16.32099

S	16.33432	13.02676	9.15979
S	9.10514	16.30832	12.89774
S	14.84744	7.58400	12.72365
S	12.68791	14.81746	7.54709
S	7.62468	12.66614	14.83224
S	7.56275	11.10249	9.19972
S	9.33784	7.52864	11.12029
S	11.12656	9.25240	7.53515
S	15.27676	14.03587	17.66339
S	17.70020	15.30960	14.05962
S	13.99251	17.67662	15.25721
S	8.82408	9.73855	17.67363
S	17.39804	8.85359	9.62873
S	9.74752	17.67823	8.79027
S	10.02551	6.17767	15.15436
S	15.18557	9.94835	6.42402
S	6.19649	15.10918	10.00273
S	6.32971	8.57785	14.04986
S	14.11212	6.15124	8.47441
S	8.60221	14.06242	6.27771
C	10.70824	13.40569	17.63373
C	17.60416	10.70399	13.31021
C	13.39936	17.65815	10.70702
C	10.81362	13.69938	19.01343
C	18.99939	10.79356	13.52646
C	13.68541	19.03831	10.81636
H	11.26396	14.65561	19.34043
H	19.38524	11.24525	14.45983
H	14.63608	19.36803	11.27652
C	10.33017	12.76632	19.95105
C	19.88059	10.29268	12.54917
C	12.75106	19.97076	10.32479
H	10.41350	12.99205	21.03308
H	20.97386	10.35553	12.72295
H	12.96784	21.05451	10.40952
C	9.74015	11.55808	19.53944
C	19.40261	9.70217	11.36442
C	11.55281	19.55257	9.71970
H	9.34821	10.83887	20.28416
H	20.10714	9.28891	10.61693
H	10.83119	20.29310	9.32440
C	9.63992	11.24797	18.15751
C	18.00539	9.62711	11.12552
C	11.25032	18.16917	9.61672

C	10.14598	12.17840	17.22375
C	17.13121	10.14569	12.10392
C	12.17959	17.24106	10.13359
H	10.07230	11.94360	16.14168
H	16.03799	10.09482	11.92406
H	11.95012	16.15718	10.06355
C	13.35315	10.39349	17.53094
C	17.56391	13.48371	10.37672
C	10.35272	17.52332	13.32867
C	13.19312	10.09202	18.90312
C	18.93789	13.31505	10.08249
C	10.05456	18.89416	13.15228
H	12.71184	9.14295	19.20591
H	19.25205	12.88251	9.11173
H	9.10949	19.19292	12.66106
C	13.66156	11.00741	19.86446
C	19.90432	13.72384	11.02055
C	10.97074	19.85988	13.61267
H	13.54092	10.77135	20.94054
H	20.97872	13.57863	10.78999
H	10.73912	20.93526	13.47599
C	14.28793	12.20753	19.48323
C	19.52432	14.31335	12.23818
C	12.16890	19.48461	14.24469
H	14.66819	12.91382	20.24584
H	20.29004	14.64581	12.96509
H	12.87346	20.25162	14.62021
C	14.43512	12.52856	18.10857
C	18.14912	14.49139	12.54563
C	12.48938	18.11093	14.40474
C	13.94877	11.61360	17.15019
C	17.18767	14.05439	11.60893
C	11.57231	17.14854	13.93024
H	14.05904	11.85847	16.07329
H	16.11111	14.17685	11.84740
H	11.81135	16.07273	14.05980
C	13.59261	6.36296	13.11132
C	13.13405	13.51925	6.39176
C	6.40684	13.07096	13.58044
C	12.42009	6.72548	13.80229
C	13.81585	12.35805	6.81199
C	6.76301	13.74751	12.39522
H	12.22345	7.79254	14.03114
H	13.99797	12.19744	7.89399

H	7.83102	13.95961	12.18416
C	11.47965	5.75606	14.21788
C	14.27142	11.39191	5.88942
C	5.78906	14.18096	11.46980
C	11.73329	4.39458	13.90712
C	14.02008	11.59964	4.50964
C	4.42550	13.90186	11.74710
H	11.00416	3.62495	14.22671
H	14.36821	10.84988	3.77357
H	3.65018	14.23474	11.03069
C	12.88967	4.03581	13.19152
C	13.30997	12.74023	4.09186
C	4.07114	13.20084	12.91306
H	13.06780	2.97089	12.94052
H	13.08799	12.88288	3.01574
H	3.00504	12.97060	13.10959
C	13.82677	5.00611	12.78757
C	12.86438	13.70430	5.01648
C	5.04732	12.78160	13.83745
H	14.73630	4.72219	12.22463
H	12.30906	14.60097	4.68176
H	4.76476	12.23175	14.75477
C	6.37642	10.55085	10.42900
C	10.52655	6.32515	10.53015
C	10.58826	10.45658	6.32640
C	6.78264	9.98692	11.65708
C	11.74895	6.69146	9.92581
C	10.02134	11.68327	6.72826
H	7.85856	9.98054	11.93282
H	12.05675	7.75764	9.90527
H	10.01918	11.96623	7.80206
C	5.85159	9.39776	12.54064
C	12.58419	5.72360	9.32071
C	9.42319	12.55783	5.79376
C	4.47745	9.41412	12.18500
C	12.19224	4.36413	9.34743
C	9.43338	12.19007	4.42175
H	3.73741	8.95302	12.86696
H	12.84130	3.60710	8.86630
H	8.95834	12.86027	3.67938
C	4.06799	10.00989	10.97959
C	10.98999	3.99482	9.97807
C	10.03523	10.98462	4.01734
H	2.99119	10.02579	10.71676

H	10.68985	2.92839	10.00078
H	10.04007	10.70936	2.94336
C	5.00269	10.57665	10.09179
C	10.15471	4.95945	10.56874
C	10.61246	10.10835	4.95625
H	4.67874	11.02790	9.13474
H	9.20208	4.66744	11.04919
H	11.06424	9.14840	4.64323
Na	17.40195	10.90581	7.78562

3. Lowest energy structure of $[Ag_{29}(BDT)_{12}Na]_2^{4-}$

Ag	12.37740	11.69433	12.00183
Ag	13.09149	13.06790	14.42051
Ag	11.53374	14.41782	12.41534
Ag	10.40224	12.30024	13.97578
Ag	12.34086	10.04092	14.29241
Ag	14.35750	13.66263	11.85953
Ag	9.88713	12.46379	10.85814
Ag	15.01878	11.02061	12.90129
Ag	12.30643	13.24506	9.60731
Ag	10.40273	9.67892	12.22666
Ag	11.51317	10.50176	9.56700
Ag	13.13167	8.94680	11.78442
Ag	14.52717	11.29915	10.12577
Ag	12.26712	14.99767	16.62078
Ag	10.82666	16.55726	14.45720
Ag	9.38106	14.40261	15.97002
Ag	14.67471	10.97350	15.86698
Ag	13.30199	15.98868	10.47896
Ag	7.91855	11.27272	12.73833
Ag	11.84838	7.21985	15.36786
Ag	16.91182	12.75226	11.29963
Ag	8.30205	12.83292	8.28742
Ag	18.48773	10.88218	12.80063
Ag	10.83818	13.87899	7.00315
Ag	9.64728	6.89911	13.33812
Ag	12.39797	6.02333	12.63187
Ag	17.74090	10.95525	9.28824
Ag	10.14958	10.96003	6.82860
Ag	13.71213	8.62526	8.90180
S	8.10963	12.19000	15.09673
S	14.46873	13.41894	16.53441
S	11.38345	16.90917	11.85213

S	12.92725	9.28248	16.64680
S	15.67710	15.85016	11.48309
S	7.35730	12.82092	10.80429
S	16.72168	10.09668	14.55640
S	12.90730	15.19916	8.09438
S	8.02511	8.77476	12.34006
S	11.51281	8.81672	7.65645
S	13.97725	6.81907	10.64514
S	15.60005	10.09999	8.13240
S	10.50904	14.09873	18.18729
S	12.67388	17.37292	15.94728
S	8.36487	16.46284	14.93215
S	9.42015	6.78584	15.84298
S	18.79514	13.49845	13.00439
S	8.65507	15.11024	7.30455
S	13.56686	5.48007	14.76088
S	18.13240	13.42029	8.97476
S	7.66668	10.70472	7.09697
S	10.25072	5.11487	11.68481
S	18.92691	9.34769	10.76394
S	11.43821	12.31078	5.14117
C	8.15814	10.70698	16.10608
C	16.03690	14.10895	15.99861
C	10.03683	17.04414	10.67276
C	7.42946	10.69752	17.31908
C	16.70408	15.02430	16.84498
C	9.23650	18.21090	10.69193
H	6.94250	11.62662	17.67185
H	16.21065	15.37150	17.77228
H	9.38830	18.96561	11.48638
C	7.33117	9.49890	18.05166
C	18.00001	15.45803	16.50535
C	8.26974	18.39797	9.68532
H	6.75490	9.48696	18.99907
H	18.53167	16.16226	17.17588
H	7.64557	19.31453	9.69518
C	7.94012	8.31554	17.59833
C	18.64325	15.00055	15.34084
C	8.08969	17.44946	8.66294
H	7.84577	7.37357	18.17272
H	19.67156	15.33272	15.10292
H	7.34147	17.61377	7.86332
C	8.69489	8.31713	16.39565
C	17.97231	14.10084	14.47473

C	8.87328	16.26590	8.64444
C	8.80111	9.52732	15.67318
C	16.67225	13.67389	14.81690
C	9.83029	16.07736	9.66635
H	9.39141	9.53966	14.73341
H	16.14811	12.96339	14.14507
H	10.44810	15.15501	9.65719
C	11.82713	10.21879	17.71118
C	15.52210	16.74189	13.03049
C	7.11569	14.41985	11.57588
C	11.31170	9.58857	18.86784
C	16.56426	17.60118	13.45533
C	6.10874	15.27389	11.06672
H	11.51404	8.51534	19.04481
H	17.49013	17.70096	12.85459
H	5.55969	14.98769	10.14915
C	10.55944	10.34681	19.78494
C	16.40992	18.34731	14.63981
C	5.82015	16.47321	11.74538
H	10.15951	9.85556	20.69452
H	17.23062	19.01364	14.97326
H	5.03471	17.14612	11.34579
C	10.31375	11.71492	19.57169
C	15.23238	18.26202	15.40264
C	6.51005	16.83440	12.91602
H	9.73890	12.30868	20.30825
H	15.11836	18.85709	16.32946
H	6.26686	17.77380	13.44905
C	10.80417	12.35244	18.40234
C	14.17957	17.40401	14.99036
C	7.53695	15.99619	13.42463
C	11.54945	11.58236	17.48132
C	14.35197	16.64252	13.81437
C	7.83057	14.80150	12.73078
H	11.93848	12.07353	16.56515
H	13.53654	15.95964	13.49671
H	8.63196	14.14106	13.12222
C	16.55540	8.30966	14.55895
C	14.53765	14.77369	7.47249
C	7.55622	8.56818	10.62165
C	15.28830	7.69140	14.54038
C	15.53138	14.24633	8.32464
C	7.85128	9.54820	9.65036
H	14.37344	8.31043	14.43257

H	15.27157	14.00953	9.37596
H	8.46515	10.42882	9.93066
C	15.15079	6.29066	14.67141
C	16.85004	14.01900	7.87506
C	7.37922	9.44428	8.32324
C	16.32335	5.49930	14.78205
C	17.16952	14.32882	6.52850
C	6.60969	8.30480	7.96949
H	16.22724	4.39992	14.86834
H	18.19755	14.15617	6.15755
H	6.24064	8.20484	6.93023
C	17.58771	6.11252	14.77179
C	16.17351	14.83232	5.67089
C	6.33806	7.31258	8.92825
H	18.50070	5.48793	14.84131
H	16.42855	15.05484	4.61615
H	5.75133	6.41805	8.63601
C	17.71653	7.51040	14.67406
C	14.86009	15.05637	6.12584
C	6.79980	7.43078	10.25370
H	18.71533	7.98119	14.70443
H	14.08087	15.44810	5.44428
H	6.58736	6.64794	11.00639
C	10.60987	7.38911	8.25914
C	15.74949	6.75708	10.88700
C	15.00519	10.90244	6.64593
C	10.68458	6.96140	9.60270
C	16.53402	7.92673	10.81977
C	13.67534	11.35963	6.54812
H	11.23176	7.57693	10.34704
H	16.03953	8.91582	10.73005
H	13.01631	11.32403	7.44093
C	10.10323	5.74429	10.02431
C	17.94176	7.86262	10.84561
C	13.14848	11.83389	5.32676
C	9.41154	4.95835	9.06588
C	18.57047	6.59858	10.95731
C	14.00692	11.89053	4.19869
H	8.95624	4.00039	9.38361
H	19.67619	6.53264	10.97665
H	13.61043	12.26567	3.23589
C	9.30769	5.39862	7.73502
C	17.78674	5.43466	11.05321
C	15.34556	11.47068	4.30669

H	8.75451	4.78116	6.99888
H	18.28877	4.45174	11.14824
H	16.01148	11.53026	3.42317
C	9.90096	6.60520	7.31779
C	16.38168	5.49840	11.02094
C	15.85578	10.96793	5.51846
H	9.83344	6.94352	6.26669
H	15.76989	4.57848	11.08585
H	16.90058	10.61143	5.59503
Na	18.52227	15.41837	10.95586
Ag	27.85165	12.33035	11.93239
Ag	26.95021	10.71180	14.13698
Ag	28.44921	9.52188	11.98025
Ag	29.70018	11.30674	13.82961
Ag	27.95002	13.65727	14.44207
Ag	25.71956	10.58302	11.46362
Ag	30.30109	11.52281	10.73684
Ag	25.26700	13.11245	12.86596
Ag	27.87571	11.13843	9.32856
Ag	29.96942	14.13590	12.47516
Ag	28.88183	13.77843	9.71267
Ag	27.30637	15.13081	12.09205
Ag	25.83933	13.19603	10.07281
Ag	27.53116	8.44085	16.05378
Ag	28.89095	7.05943	13.73412
Ag	30.47590	8.88585	15.52789
Ag	25.49283	12.73667	15.82313
Ag	26.67981	8.41017	9.74762
Ag	32.30319	12.29241	12.78885
Ag	28.60067	16.28160	15.91409
Ag	23.33908	11.92684	10.94994
Ag	31.95919	11.38201	8.17248
Ag	21.77617	13.64367	12.71506
Ag	29.39867	10.76281	6.69364
Ag	30.88555	16.63952	13.97717
Ag	28.21509	17.83678	13.35100
Ag	22.56799	13.97161	9.15507
Ag	30.32311	13.59797	6.96312
Ag	26.85474	15.91778	9.26638
S	31.94782	11.08697	14.99704
S	25.50024	10.20892	16.18826
S	28.42737	7.14049	11.07149
S	27.34860	14.12906	16.87328
S	24.31371	8.55692	10.71665

S	32.78368	10.94774	10.68433
S	23.55373	13.90825	14.58951
S	27.18809	9.49442	7.50964
S	32.41709	14.82492	12.74611
S	29.07624	15.69659	8.05455
S	26.55441	17.42085	11.26779
S	24.87083	14.71892	8.24517
S	29.32261	8.97015	17.74612
S	26.93257	6.22233	15.05370
S	31.33543	6.88785	14.25612
S	31.04786	16.41347	16.48040
S	21.41001	11.08390	12.50418
S	31.44625	9.29702	6.87865
S	27.01307	18.19823	15.50647
S	22.10252	11.56588	8.56264
S	32.80485	13.59580	7.30234
S	30.44987	18.68759	12.59130
S	21.37389	15.33866	10.85651
S	28.96857	12.63367	5.07655
C	31.97602	12.40312	16.21575
C	23.91254	9.74689	15.48513
C	29.79871	7.04543	9.91675
C	32.65801	12.17589	17.43480
C	23.11082	8.78458	16.14005
C	30.50075	5.82294	9.79307
H	33.05990	11.16945	17.65940
H	23.50282	8.25555	17.02943
H	30.26185	4.98123	10.47061
C	32.82063	13.24320	18.33901
C	21.81447	8.52364	15.65268
C	31.48443	5.69584	8.79318
H	33.35479	13.06711	19.29498
H	21.18099	7.76969	16.16091
H	32.03427	4.73858	8.68851
C	32.32411	14.52649	18.04858
C	21.30061	9.21525	14.54170
C	31.77575	6.75620	7.91695
H	32.46636	15.36257	18.75999
H	20.28020	9.01573	14.16144
H	32.53928	6.63853	7.12375
C	31.61973	14.76186	16.83837
C	22.09818	10.18173	13.87972
C	31.08905	7.99269	8.04100
C	31.44254	13.68122	15.94573

C	23.40404	10.41482	14.35242
C	30.11611	8.11825	9.05658
H	30.88566	13.85684	15.00165
H	24.03777	11.15900	13.82918
H	29.57338	9.08046	9.16167
C	28.32979	12.96688	17.82446
C	24.30912	7.46166	12.13027
C	32.87020	9.24490	11.23909
C	28.84989	13.37889	19.07391
C	23.17398	6.65955	12.39796
C	33.82838	8.38537	10.65165
H	28.72291	14.42726	19.40427
H	22.27447	6.72751	11.75438
H	34.43660	8.74370	9.79925
C	29.51406	12.43795	19.88395
C	23.19929	5.76336	13.48360
C	33.99157	7.08578	11.16882
H	29.92388	12.75903	20.86268
H	22.30599	5.14309	13.69523
H	34.73805	6.40815	10.70739
C	29.66541	11.10101	19.47491
C	24.33779	5.64395	14.29967
C	33.22517	6.63050	12.25599
H	30.17479	10.36425	20.12586
H	24.35283	4.93063	15.14538
H	33.36678	5.60957	12.66019
C	29.16403	10.68234	18.21509
C	25.48164	6.44347	14.04316
C	32.24957	7.47792	12.84468
C	28.51175	11.63442	17.40217
C	25.44113	7.35177	12.96442
C	32.08072	8.77425	12.30997
H	28.11813	11.31204	16.41649
H	26.32945	7.98565	12.76495
H	31.31845	9.44113	12.76361
C	23.84335	15.65743	14.84141
C	25.60738	10.12837	6.94057
C	32.95146	15.23459	11.08276
C	25.14883	16.17001	14.97609
C	24.64095	10.61939	7.84441
C	32.61710	14.41977	9.98109
H	26.02055	15.49632	14.84432
H	24.88806	10.68527	8.92340
H	31.92610	13.56384	10.12508

C	25.37683	17.53034	15.27673
C	23.35879	11.02145	7.41084
C	33.15036	14.65409	8.69453
C	24.25941	18.39052	15.42803
C	23.04833	10.92792	6.02987
C	34.02849	15.75612	8.52215
H	24.42647	19.45984	15.65912
H	22.04910	11.24039	5.67153
H	34.45229	15.95694	7.51934
C	22.95755	17.88574	15.26415
C	24.01595	10.45275	5.12589
C	34.33522	16.59150	9.61086
H	22.08999	18.56698	15.36205
H	23.76945	10.39581	4.04742
H	35.00264	17.46366	9.45611
C	22.73616	16.52772	14.97121
C	25.29301	10.05360	5.56453
C	33.80675	16.34541	10.89294
H	21.70922	16.13756	14.83604
H	26.05183	9.68713	4.84724
H	34.04576	17.00806	11.74643
C	30.06702	16.94775	8.87248
C	24.77625	17.57365	11.45042
C	25.45512	14.08966	6.67165
C	29.96437	17.19553	10.25781
C	23.89081	16.50013	11.21472
C	26.75229	13.54948	6.54883
H	29.33290	16.53545	10.88842
H	24.29399	15.48472	11.01885
H	27.37497	13.40652	7.45654
C	30.62584	18.28573	10.86475
C	22.49067	16.69946	11.20392
C	27.29337	13.21239	5.28850
C	31.42687	19.12869	10.05072
C	21.97533	17.99277	11.45667
C	26.48395	13.39043	4.13671
H	31.94655	19.98782	10.51750
H	20.88043	18.16203	11.44001
H	26.89624	13.12979	3.14282
C	31.55333	18.86715	8.67510
C	22.85892	19.05596	11.72513
C	25.17605	13.89226	4.26278
H	32.18330	19.53021	8.04813
H	22.44971	20.06392	11.93526

H	24.55036	14.02066	3.35694
C	30.88220	17.78505	8.07438
C	24.25145	18.85980	11.72500
C	24.65051	14.24959	5.51944
H	30.97197	17.58540	6.98990
H	24.94307	19.69991	11.92544
H	23.63033	14.66710	5.61340
Na	21.64199	9.35531	10.27244