Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Silver cation tagged on 5,7,12,14-tetraphenyl-6,13-diazapentacene and its dihydro-form

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Contents

1) Isotope pattern of selected signals

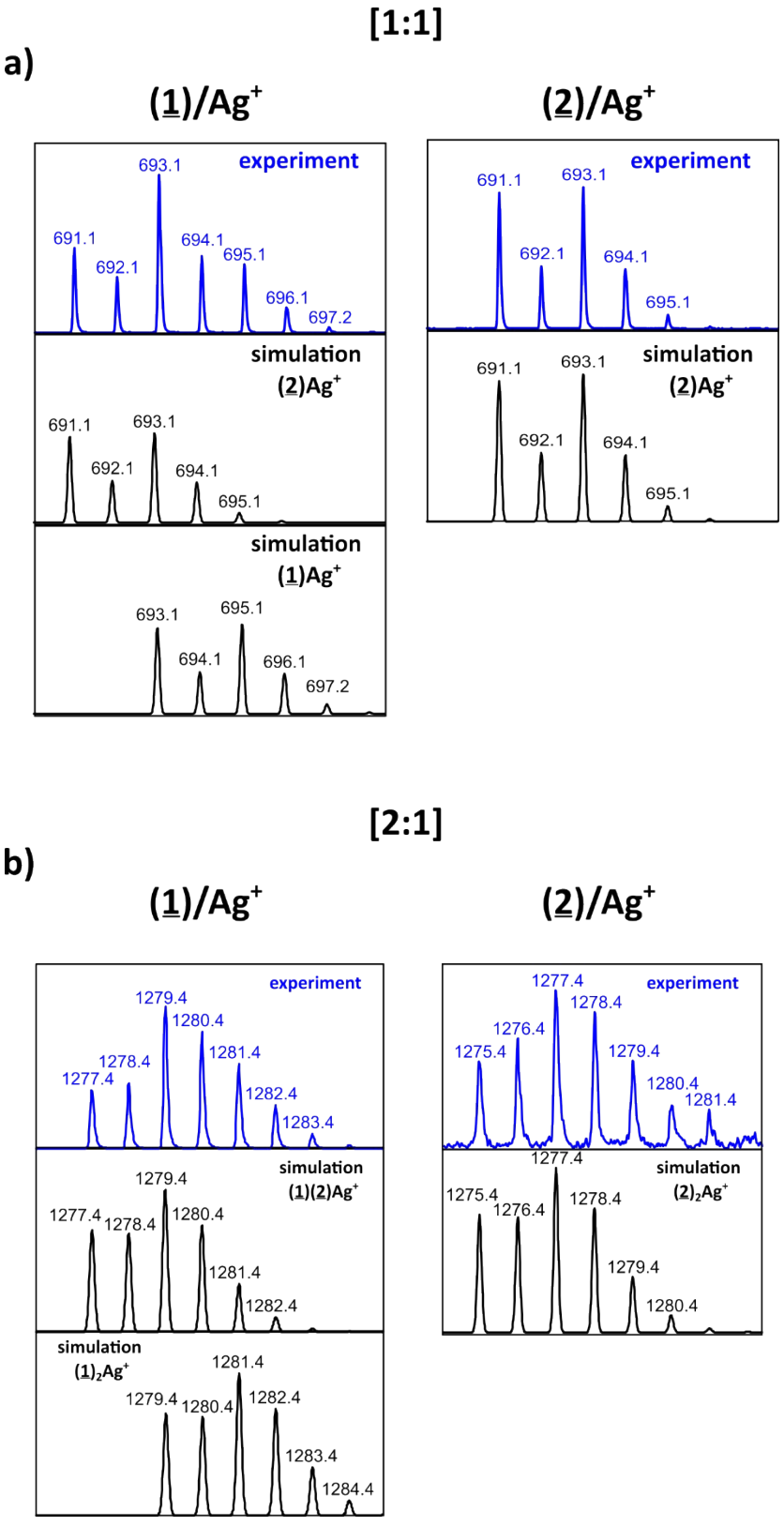


Figure S1: Isotope Pattern of analyte solution **1**/Ag⁺ and **2**/Ag⁺ of a) the 1:1 complexes and b) the 2:1 complexes. Due to the oxidation of **1** into **2** in the analyte solution, the isotope pattern of both complexes overlap.

2) Additional mass spectra

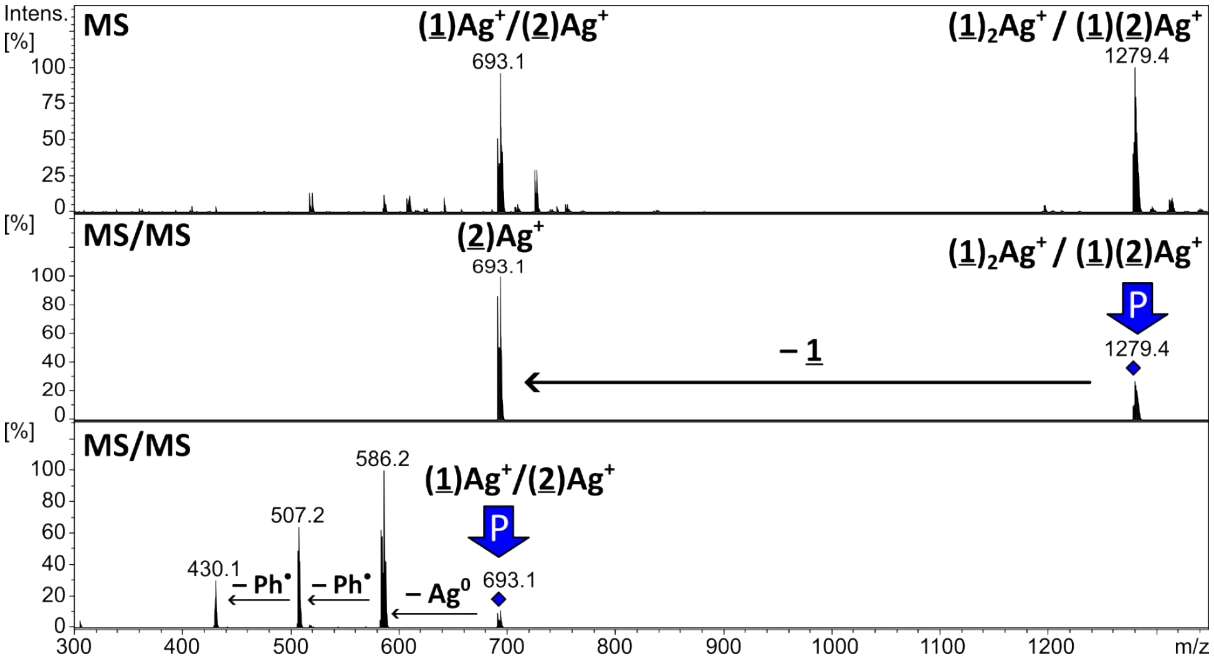
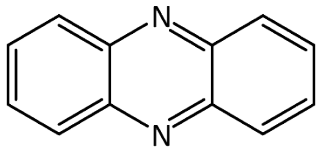


Figure S2: MS and MS/MS of the analyte **1**/Ag⁺. The 2:1 complex of (**1**)$_2$Ag⁺ and (**1**)(**2**)Ag⁺ both dissociate by the loss of a neutral **1**. The 1:1 complexes (**1**)Ag⁺ and (**2**)Ag⁺ dissociated at distinctly different collision energies and can therefore be easily identified.



P = $C_{12}H_8N_2$

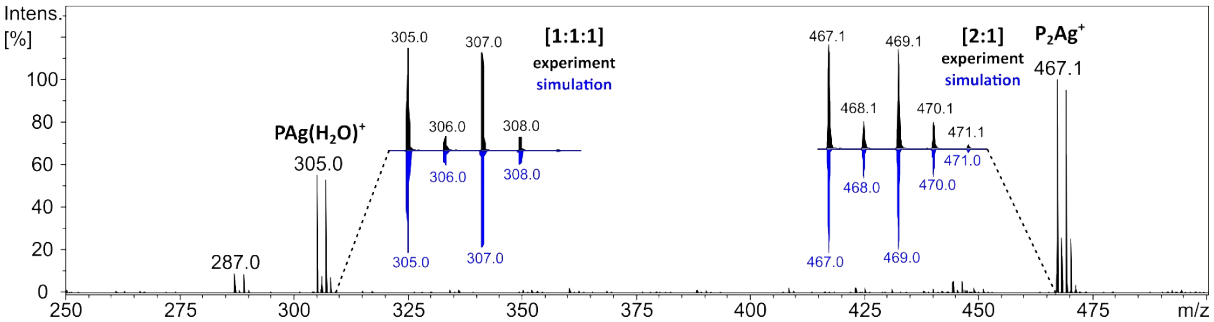
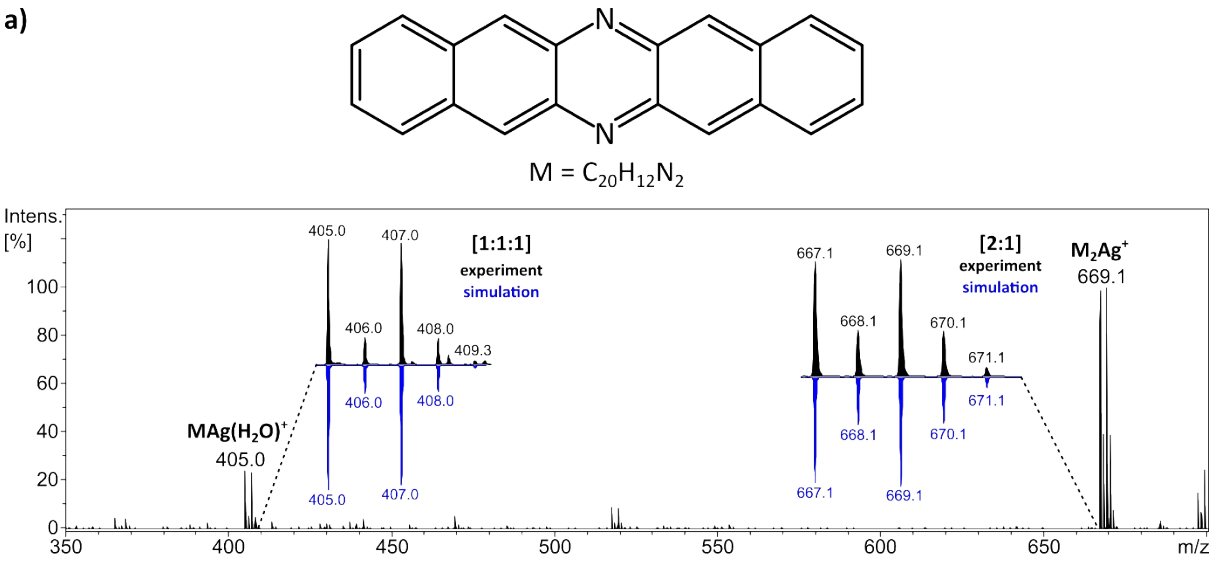


Figure S3: MS of phenazine (P) in the presence of Ag⁺. No 1:1 complex could be detected, the electron demand of Ag⁺ leads to the addition to an additional H_2O molecule to form a 1:1:1 complex. For the 2:1 complex, the second phenazine satisfies the electron demand of the Ag⁺.

a)



b)

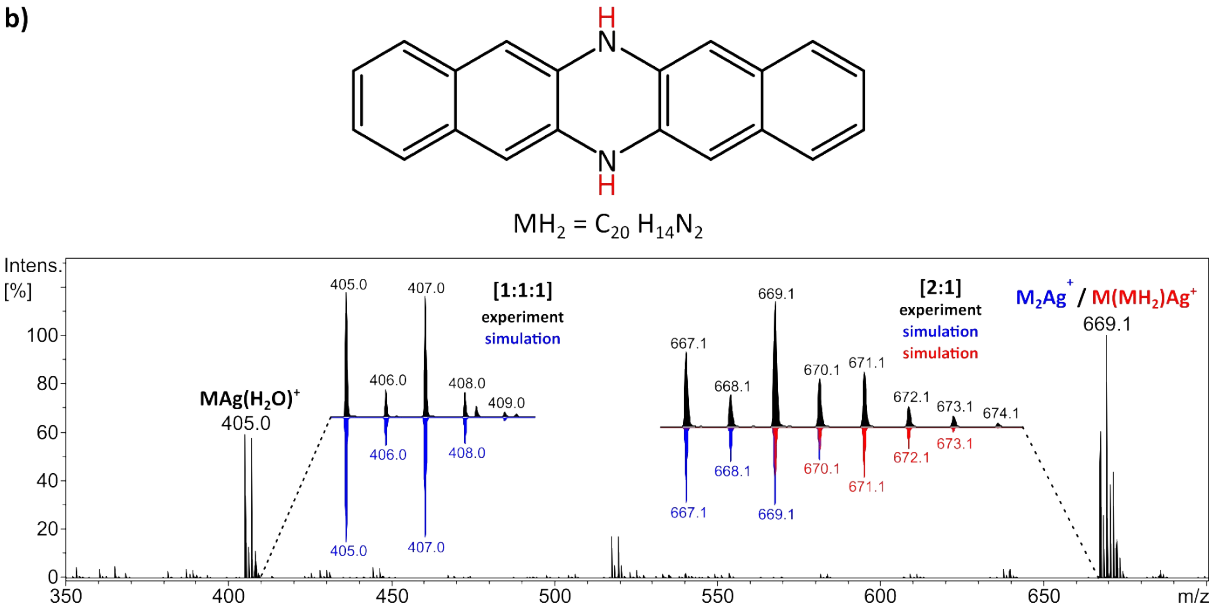


Figure S4: MS of a) diazapentacene (M) and b) dihydro-diazapentacene (MH_2) in the presence of Ag^+. No 1:1 complex could be detected, the electron demand of Ag^+ leads to the addition to an additional H_2O molecule to form a 1:1:1 complex. For the 2:1 complex, the second diazapentacene satisfies the electron demand of the Ag^+. As we have seen for molecule **1** and **2**, the 2:1 complex of MH_2 composes of a homoleptic M_2Ag^+ and a heteroleptic $M(MH_2)Ag^+$ complex.

3) Changing complex isotope pattern with ongoing reaction time

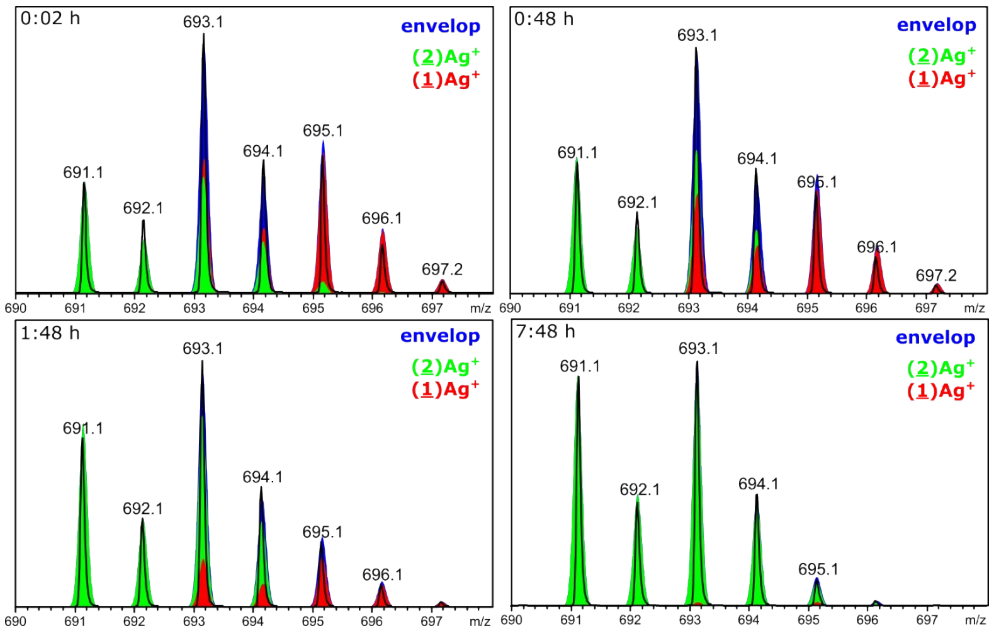


Figure S5: Isotope pattern of the overlapping signals (**1**)Ag^+ and (**2**)Ag^+. With ongoing oxidation of **1** into **2**, the isotope pattern of (**1**)Ag^+ diminishes until (almost) only the signal of (**2**)Ag^+ remains. After 7:48h **1** is fully oxidized and only the complex signal of (**2**)Ag^+ could be detected.

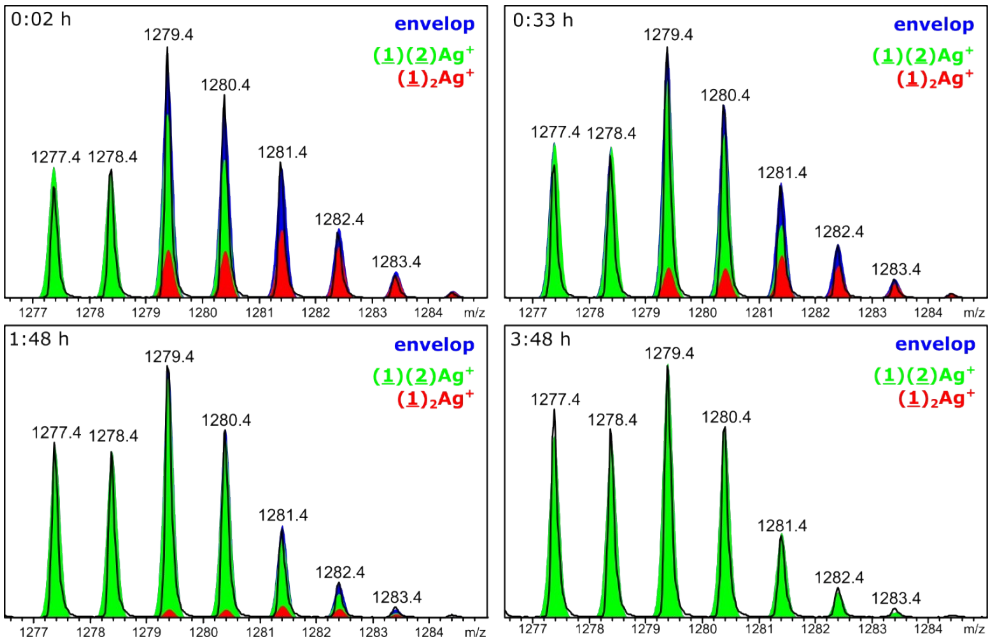


Figure S6: Isotope pattern of the overlapping signals (**1**)(**2**)Ag^+ and (**1**)$_2Ag^+$. With ongoing oxidation of **1** into **2**, the isotope pattern of (**1**)$_2Ag^+$ diminishes until (almost) only the signal of (**1**)(**2**)Ag^+ remains. After 3:48h only the complex signal of (**1**)(**2**)Ag^+ could be detected.

4) Breakdown-graphs of the mixed complexes

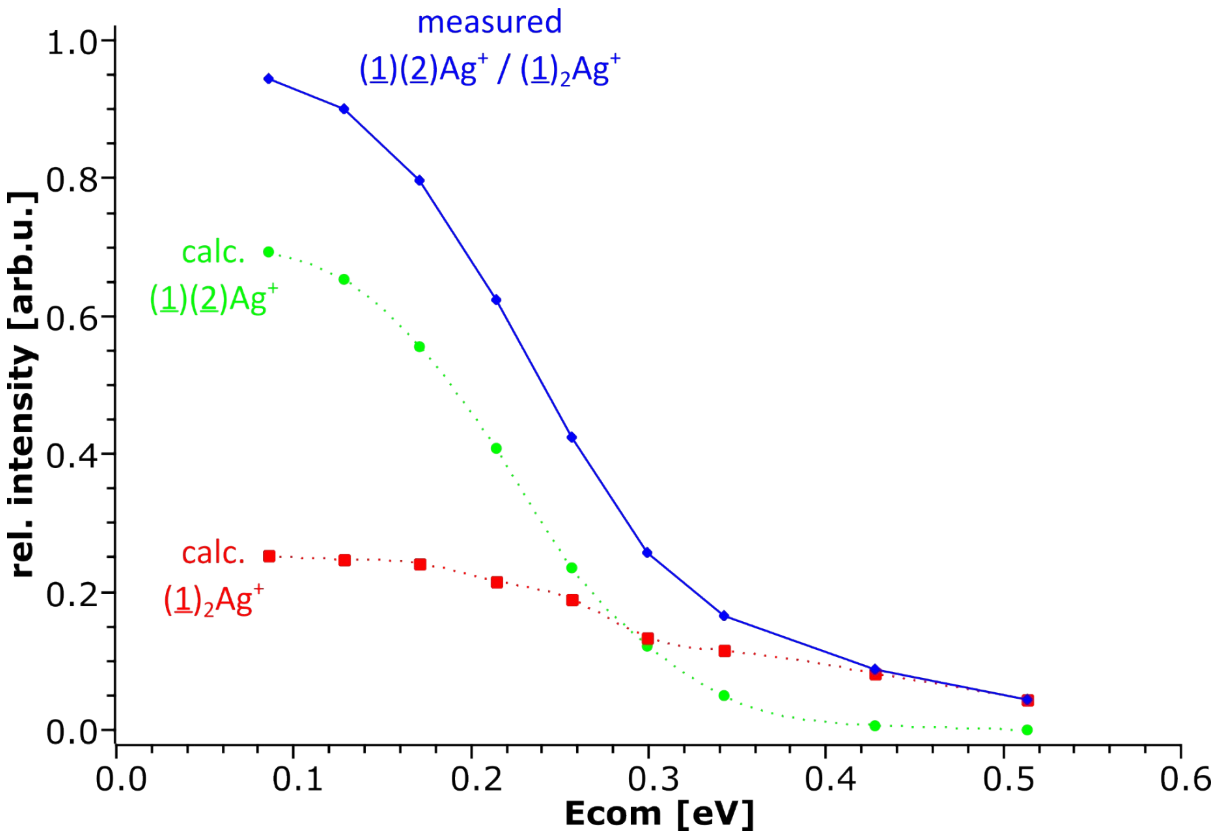


Figure S7: Calculated breakdown graphs of (**1**)(**2**)Ag^+ and (**1**)$_2Ag^+$ extracted from the changing isotope patter (see 5.2) of the measured mixed signal.

5) Determination of the reaction order

5.1) Determination of the reaction progress from the breakdown graph

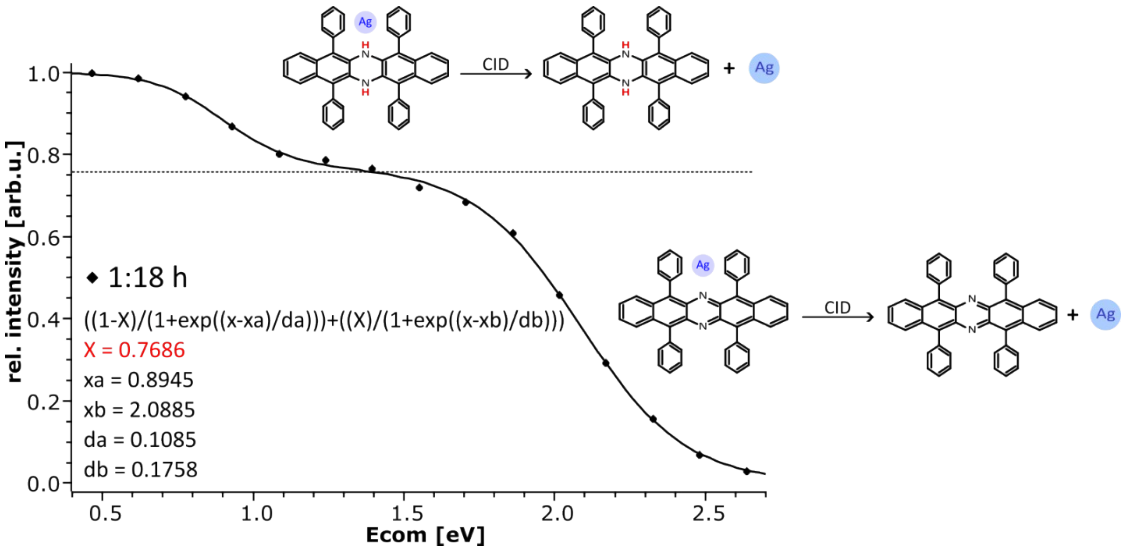


Figure S8: The reaction progress was tracked from the changing appearance of the breakdown graph of the 1:1 complex from the **1**/Ag^+ analyte solution. The (**1**)Ag^+ complex dissociated at distinctly lower collision energies than (**2**)Ag^+, this leads to a breakdown graph with a plateau in the middle. The first decline in rel. intensity is due to the dissociation of (**1**)Ag^+, while the (**2**)Ag^+ complex stays intact. The second intensity drop is caused by the dissociation of (**2**)Ag^+. Hence, the position of the plateau indicates the amount of **1** and **2** in the analyte solution. The curve is fitted as a double sigmoid Boltzmann function.

Table S1: Amount of (**1**)Ag^+ and (**2**)Ag^+ in the analyte solution **1**/Ag^+, extracted from the breakdown graphs of the 1:1 complex.

reaction time [h]	(1)Ag^+ [%]	(2)Ag^+ [%]
0:18	39.9	60.1
0:33	35.2	64.8
0:48	30.5	69.5
1:18	23.1	76.9
1:48	17.6	82.4
2:48	9.7	90.3
3:48	6.7	93.3
4:48	3.6	96.4
5:58	1.7	98.3
6:48	1.6	98.4
7:48	1.4	98.9

5.2) Determination of the reaction progress from the isotope pattern

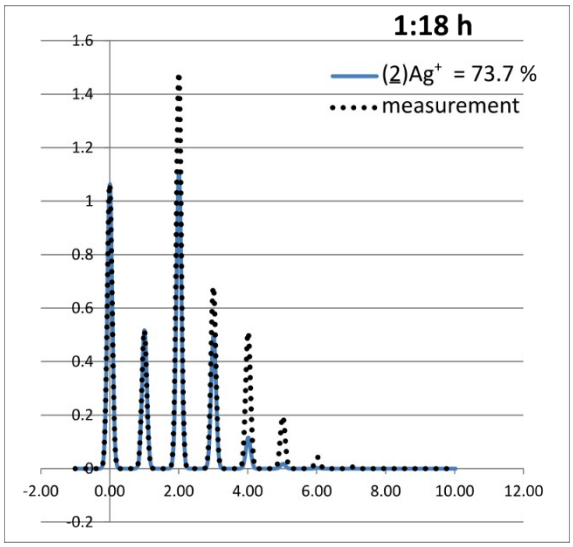


Figure S9: Example of the extraction of the reaction progress from the isotope pattern. Due to the two additional hydrogen atoms, the isotope pattern of **1** is shifted by two mass units compared to the isotope pattern of **2**. Therefore the first to peaks of the pattern belong exclusively to the (**2**)Ag^+ complex. Based on the intensity of those first two peaks, one can calculate the amount of (**2**)Ag^+ from the overlapping peaks. In the example shown, the black dotted line represents the measured mixed isotope pattern. The calculated amount of (**2**)Ag^+ from the complex amounts to 73.7%, therefore the remaining 26.3% are assigned to (**1**)Ag^+.

Table S2: Amount of (**1**)Ag^+ and (**2**)Ag^+ in the analyte solution **1**/Ag^+, extracted from the isotope pattern of the 1:1 complex.

reaction time [h]	(1)Ag^+ [%]	(2)Ag^+ [%]
0:18	47.2	52.8
0:33	44.2	55.8
0:48	42.2	57.8
1:18	26.3	73.7
1:48	20.8	79.2
2:48	11.2	88.8
3:48	6.2	93.8
4:48	6.9	93.1
5:58	2.7	97.3
6:48	2.7	97.3
7:48	1.8	98.2

5.3) Determination of the reaction order in day light

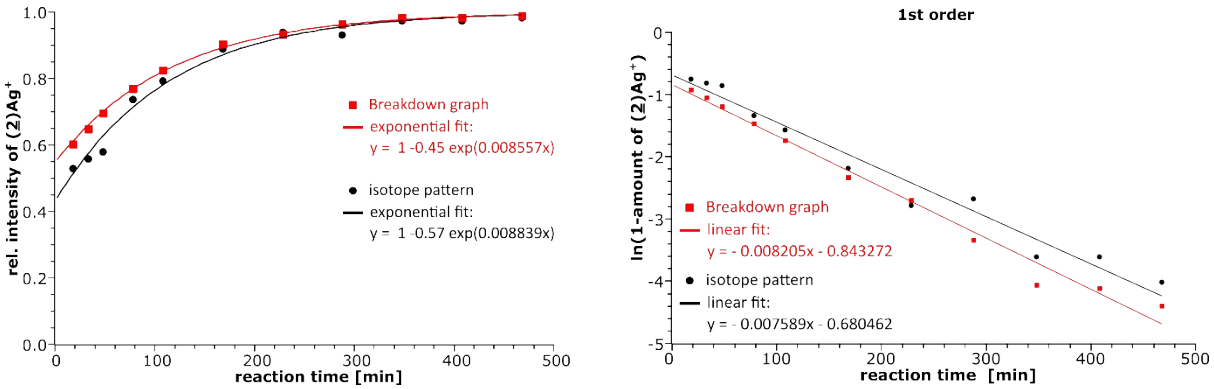


Figure S10: To determine the reaction order, the calculated amount of (**2**)Ag^+ from the breakdown graph and the isotope pattern analysis were plotted as a function of the reaction time (left plot). For both methods, an exponential correlation between the amount of (**2**)Ag^+ and the reaction time could be determined, this points to a first order reaction. The logarithm of the (**2**)Ag^+ abundance was also plotted against the reaction time (right plot). Here a linear relationship could be obtained, confirming the assumed first order reaction. The rate constant could be determined as -0.008215 min^{-1} and as -0.008381 min^{-1} for the isotope pattern and the breakdown graph analysis, respectively.

Table S3: determined rate constants from the isotope pattern and breakdown graph analysis measured in (ambient) day light.

DAY LIGHT	isotope pattern	breakdown graph
k (exponential fit) [min^{-1}]	- 0.008839 ± 0.000560	- 0.008557 ± 0.000267
k (linear fit) [min^{-1}]	- 0.007589 ± 0.000396	- 0.008205 ± 0.000303

5.4) Determination of the reaction order in the dark

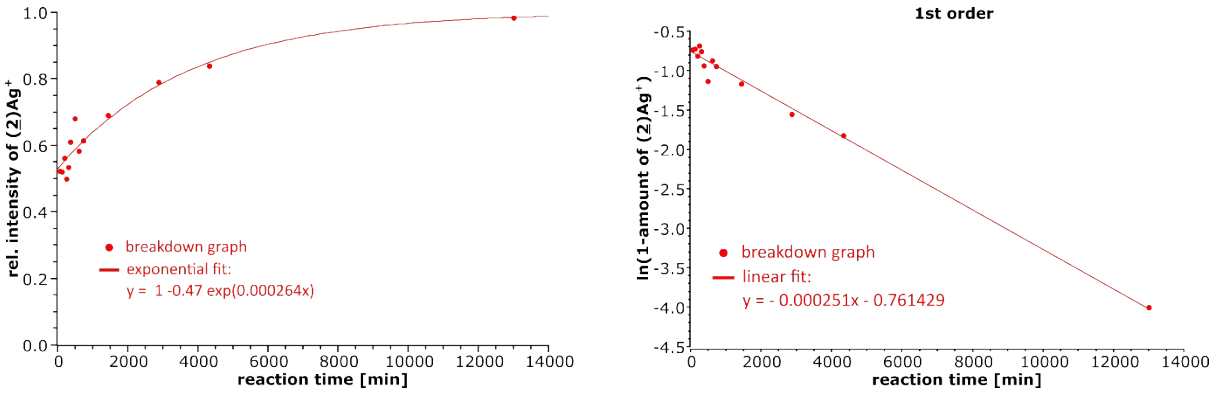


Figure S11: Also for the measurements performed in the dark the calculated abundance of the (**2**)Ag^+ complex was plotted against the reaction time (left plot). The data abstracted from the isotope pattern analysis showed such a large deviation that no reliable assessment could be made from them, so they would not be considered further. The data from the breakdown graph analysis showed also an exponential behavior. The assumed first order reaction is confirmed by the logarithm plot of the (**2**)Ag^+ abundance which showed also a linear behavior. The rate constant could be determined as -0.000258 min^{-1}.

Table S4: determined rate constants from breakdown graph analysis measured in the dark.

DARK	isotope pattern	breakdown graph
k (exponential fit) [min^{-1}]	---	- 0.000264 ± 0.000019
k (linear fit) [min^{-1}]	---	- 0.000250 ± 0.000004

6. DFT calculations

6.1) calculated Ag^+–N Bond lengths

Table S5: calculated Ag^+–N Bond lengths

Molecule	Ag^+–N [Å]
(**1**)Ag^+	2.543
(**2**)Ag^+	2.347
(**1**)$_2Ag^+$	2.308; 2.409
(**2**)$_2Ag^+$	2.386; 2.387
(**1**)Ag^+(**2**)	2.370; 2.359

6.2) calculated charges

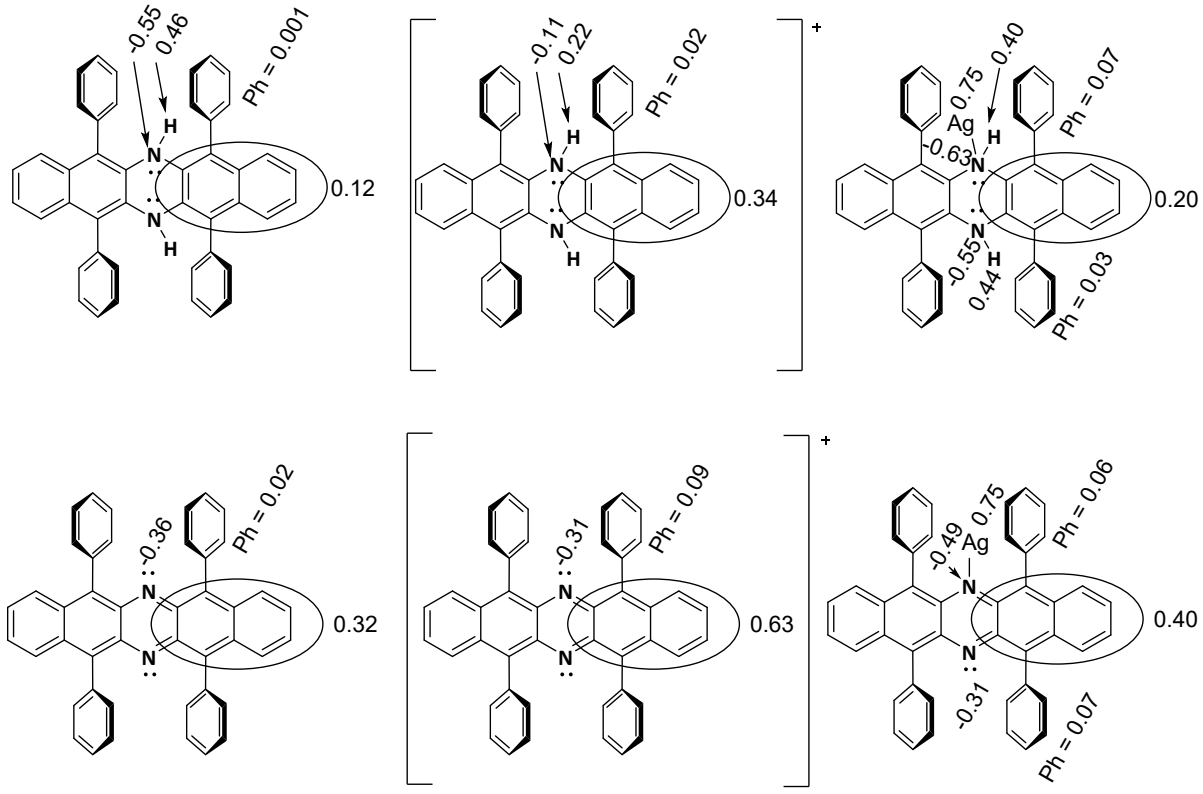


Figure S12: Interactions between both molecules and silver are of electrostatic nature. However, the calculated bond order of nitrogen to silver in (**1**)Ag^+ is slightly higher with a bond order of 0.15, when compared to the N-Ag bond in (**2**)Ag^+ with 0.09. In both cases, no covalently bonding orbital interaction was found via the calculations. For both complexes, the positive charge is predominantly located at the sliver ion with a charge of 0.75.

6.3) xyz files of the calculated structures

(**1**)

N	-1.349198	0.000091	0.001310	C	-3.595932	2.683256	-1.213807	H	2.472426	4.896178	-0.031573
N	1.349199	-0.000091	0.001320	C	-4.977033	2.551823	-1.281228	H	1.243409	7.018875	-0.025009
C	-0.711599	1.227707	0.003192	C	-5.687740	2.070363	-0.187828	H	-1.242495	7.019052	0.021831
C	-0.711767	-1.227610	-0.001738	C	-5.010745	1.731294	0.976739	H	-2.471779	4.896508	0.030106
C	0.711768	1.227611	-0.001721	C	-3.630372	1.872855	1.046089	H	-3.040876	3.045272	-2.069611
C	0.711600	-1.227707	0.003178	C	-3.596487	-2.683958	1.213686	H	-5.497824	2.817486	-2.192391
C	-1.418289	-2.410331	0.005793	C	-4.977579	-2.552381	1.281025	H	-6.762574	1.957309	-0.244467
C	-0.715142	-3.652130	0.001426	C	-5.688045	-2.069694	0.188010	H	-5.555341	1.352141	1.831475
C	0.714645	-3.652223	-0.001972	C	-5.010817	-1.729544	-0.976108	H	-3.103593	1.608426	1.954382
C	1.417958	-2.410517	-0.005381	C	-3.630459	-1.871260	-1.045392	H	-3.041621	-3.046917	2.069214
C	1.390825	-4.892326	0.012499	C	3.595931	-2.683236	-1.213847	H	-5.498550	-2.818887	2.191839
C	0.701451	-6.081645	0.009132	C	4.977032	-2.551807	-1.281266	H	-6.762870	-1.956528	0.244601
C	-1.391477	-4.892137	-0.014086	C	5.687741	-2.070373	-0.187857	H	-5.555216	-1.349416	-1.830536
C	-0.702252	-6.081546	-0.011717	C	5.010748	-1.731326	0.976718	H	-3.103505	-1.605994	-1.953339
C	1.418289	2.410332	0.005824	C	3.630374	-1.872884	1.046066	H	3.040872	-3.045233	-2.069659
C	0.715141	3.652131	0.001475	C	3.630459	1.871279	-1.045370	H	5.497821	-2.817452	-2.192436
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C	-2.902794	2.344732	-0.049580	H	1.242492	-7.019053	0.021727	H	3.041623	3.046897	2.069250
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(2)

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C	-0.723712	-1.150443	0.055896
N	-1.394361	-0.000000	-0.000003
C	1.442874	-2.374254	0.090075
C	0.728285	-3.570145	0.171853
C	-0.728292	-3.570143	0.171847
C	-1.442877	-2.374251	0.090064
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C	0.711676	-5.997113	0.392811
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C	-5.708830	-2.160192	-0.204184
C	-4.973841	-2.829062	-1.174949
C	-3.591021	-2.911756	-1.067701
C	3.591027	-2.911766	-1.067671
C	4.973849	-2.829085	-1.174903
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C	5.052354	1.572772	-0.871426
C	5.708834	2.160231	0.204154
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C	3.591020	2.911786	1.067666
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H	1.245544	6.933153	-0.494288
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H	-2.478801	4.833707	-0.321904
H	2.478794	-4.833715	0.321904
H	1.245538	-6.933159	0.494239
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H	-3.018983	-3.421343	-1.832490
H	3.018993	-3.421342	-1.832471
H	5.474745	-3.282757	-2.020676
H	6.785771	-2.090685	-0.288319
H	5.614856	-1.035314	1.623345
H	3.164750	-1.174333	1.800720
H	3.164770	1.174292	-1.800692
H	5.614872	1.035275	-1.623291
H	6.785771	2.090686	0.288361
H	5.474729	3.282796	2.020681
H	3.018980	3.421378	1.832450

(**1**)$^+$

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N	1.344280	-0.000008	0.000094
C	-0.713720	1.214954	0.006902
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C	-1.433222	-2.403014	-0.009234
C	-0.722041	-3.622351	-0.008387
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C	1.433190	-2.403031	0.009236
C	1.399315	-4.870554	0.036711
C	0.707103	-6.047552	0.023935
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C	-0.707169	-6.047543	-0.024212
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C	-0.721996	3.622359	0.008354
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C	1.399370	4.870539	-0.036830
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C	-1.399315	4.870554	0.036781
C	2.916984	2.327118	0.022224
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C	-3.618628	2.684310	-1.175611
C	-4.999249	2.545556	-1.229506
C	-5.694669	2.043022	-0.135695
C	-5.006394	1.686332	1.016866
C	-3.625763	1.829289	1.074885
C	-3.618681	-2.684398	1.175589
C	-4.999301	-2.545631	1.229480
C	-5.694698	-2.042963	0.135715
C	-5.006400	-1.686152	-1.016795
C	-3.625771	-1.829123	-1.074810
C	3.618626	-2.684296	-1.175652
C	4.999248	-2.545542	-1.229547
C	5.694669	-2.043023	-0.135730
C	5.006395	-1.686347	1.016837
C	3.625764	-1.829305	1.074856
C	3.625771	1.829138	-1.074786
C	5.006400	1.686167	-1.016774
C	5.694699	2.042964	0.135741
C	4.999302	2.545619	1.229511
C	3.618681	2.684386	1.175624
H	-2.358848	0.000016	0.000100
H	2.358849	-0.000016	0.000098
H	2.478812	-4.874865	0.074015
H	1.240608	-6.988207	0.049359
H	-2.478866	-4.874838	-0.074206
H	-1.240682	-6.988191	-0.049714
H	2.478866	4.874839	-0.074140
H	1.240682	6.988192	-0.049617
H	-1.240608	6.988206	0.049459
H	-2.478812	4.874864	0.074086
H	-3.076810	3.066749	-2.030937
H	-5.531638	2.826943	-2.128428
H	-6.769847	1.932653	-0.181132
H	-5.542199	1.299413	1.873048
H	-3.092437	1.562295	1.978924
H	-3.076881	-3.066938	2.030882
H	-5.531707	-2.827111	2.128362
H	-6.769875	-1.932584	0.181150
H	-5.542186	-1.299127	-1.872942
H	-3.092431	-1.562037	-1.978812
H	3.076807	-3.066723	-2.030982
H	5.531635	-2.826917	-2.128472
H	6.769847	-1.932654	-0.181166
H	5.542202	-1.299440	1.873024
H	3.092440	-1.562323	1.978899
H	3.092430	1.562062	-1.978791
H	5.542186	1.299152	-1.872925
H	6.769876	1.932585	0.181173
H	5.531707	2.827087	2.128397
H	3.076882	3.066914	2.030922

(**2**)$^{+}$

C	-0.704342	6.000910	-0.386786	C	2.921161	-2.329057	0.016240	H	2.473417	-4.827763	0.333363
C	0.704541	6.000887	-0.386663	C	-3.659438	1.597486	-0.953476	H	1.242066	-6.933111	0.496329
C	1.395718	4.823115	-0.284774	C	-5.040838	1.544151	-0.871478	H	-1.241816	-6.933152	0.496547
C	0.724335	3.579227	-0.149771	C	-5.706601	2.197163	0.160130	H	-2.473267	-4.827849	0.333783
C	-0.724265	3.579249	-0.149879	C	-4.982873	2.914101	1.106340	H	-3.146050	1.077889	-1.749040
C	-1.395577	4.823162	-0.285010	C	-3.600766	2.988445	1.014164	H	-5.598599	0.981675	-1.607814
C	1.450606	2.369236	-0.082565	C	-3.659437	-1.597484	0.953475	H	-6.785288	2.146708	0.227539
C	0.723586	1.150101	-0.060365	C	-5.040837	-1.544149	0.871479	H	-5.494150	3.415235	1.917458
C	-0.723636	1.150109	-0.060434	C	-5.706602	-2.197164	-0.160127	H	-3.039292	3.535856	1.759828
C	-1.450605	2.369289	-0.082769	C	-4.982874	-2.914104	-1.106336	H	-3.146048	-1.077885	1.749036
N	1.390792	-0.000000	-0.000003	C	-3.600767	-2.988447	-1.014163	H	-5.598597	-0.981672	1.607814
C	0.723586	-1.150101	0.060360	C	3.600623	-2.988361	-1.014671	H	-6.785289	-2.146709	-0.227534
C	-0.723636	-1.150109	0.060429	C	4.982694	-2.913769	-1.107201	H	-5.494152	-3.415239	-1.917453
N	-1.390840	-0.000000	-0.000003	C	5.706510	-2.196431	-0.161361	H	-3.039295	-3.535859	-1.759827
C	1.450606	-2.369236	0.082562	C	5.040869	-1.543279	0.870238	H	3.039074	-3.536052	-1.760073
C	0.724335	-3.579226	0.149770	C	3.659500	-1.596895	0.952603	H	5.493872	-3.414999	-1.918321
C	-0.724264	-3.579249	0.149877	C	3.659502	1.596896	-0.952604	H	6.785169	-2.145765	-0.229056
C	-1.450604	-2.369289	0.082766	C	5.040870	1.543280	-0.870237	H	5.598696	-0.980481	1.606277
C	1.395718	-4.823114	0.284776	C	5.706510	2.196430	0.161364	H	3.146195	-1.077163	1.748134
C	0.704541	-6.000886	0.386667	C	4.982692	2.913766	1.107204	H	3.146197	1.077166	-1.748137
C	-0.704342	-6.000909	0.386791	C	3.600622	2.988359	1.014673	H	5.598699	0.980483	-1.606277
C	-1.395577	-4.823161	0.285012	H	-1.241816	6.933154	-0.496541	H	6.785169	2.145763	0.229060
C	-2.921178	2.329250	-0.016738	H	1.242066	6.933113	-0.496322	H	5.493869	3.414995	1.918326
C	2.921161	2.329057	-0.016242	H	2.473418	4.827764	-0.333361	H	3.039071	3.536049	1.760074
C	-2.921178	-2.329250	0.016737	H	-2.473268	4.827850	-0.333780				

(**1**)Ag^+

Ag	3.057699	-0.002542	-0.886455	C	2.439810	2.401670	0.371413	H	1.521672	-0.038935	1.385701
N	-1.807445	0.005511	0.404085	C	-4.159545	-2.729455	1.120449	H	-2.928347	4.870114	-0.052941
N	0.956370	-0.015224	0.544907	C	-5.540834	-2.584442	1.096112	H	-1.701172	6.990208	-0.135945
C	0.165577	-6.066668	-0.188836	C	-6.161413	-1.986426	0.005685	H	0.777029	7.010264	0.010108
C	-1.237462	-6.031135	-0.290373	C	-5.396453	-1.540168	-1.064629	H	2.012426	4.909901	0.254333
C	-1.911024	-4.840883	-0.194224	C	-4.015999	-1.690990	-1.043677	H	-3.675986	-3.186104	1.974401
C	-1.217865	-3.622455	0.006295	C	3.128445	-2.482429	1.478665	H	-6.132027	-2.934495	1.932141
C	0.207726	-3.658951	0.092274	C	4.522270	-2.463868	1.472359	H	-7.236797	-1.868884	-0.009472
C	0.870128	-4.904958	-0.002455	C	5.223856	-2.386157	0.276786	H	-5.872415	-1.072733	-1.915955
C	-1.898009	-2.378756	0.101286	C	4.528663	-2.353451	-0.930438	H	-3.421524	-1.345816	-1.880374
C	-1.172540	-1.213671	0.275801	C	3.123856	-2.386092	-0.930668	H	2.591677	-2.549989	2.416221
C	0.241380	-1.246070	0.361767	C	3.151956	2.381545	-0.850384	H	5.060641	-2.514037	2.409510
C	0.921899	-2.438312	0.261331	C	4.556251	2.331338	-0.855313	H	6.305022	-2.374091	0.278080
C	-1.157579	1.221191	0.334472	C	5.254652	2.309833	0.350290	H	5.064052	-2.353588	-1.870784
C	0.257019	1.232129	0.419947	C	4.556904	2.350421	1.549978	H	2.580617	-2.495356	-1.862967
C	-1.865162	2.398757	0.170640	C	3.163494	2.385874	1.560884	H	2.608041	2.531730	-1.776511
C	-1.169456	3.636516	0.127289	C	-3.935951	2.534675	-1.225445	H	5.089360	2.359780	-1.796518
C	0.256032	3.652059	0.219515	C	-5.309648	2.407500	-1.384583	H	6.335587	2.284448	0.348051
C	0.953746	2.417157	0.349933	C	-6.108530	2.059804	-0.301665	H	5.098040	2.358217	2.486839
C	-1.849269	4.872310	0.001666	C	-5.529431	1.846481	0.942683	H	2.629746	2.424268	2.501797
C	-1.161209	6.057318	-0.042906	C	-4.155772	1.979498	1.103724	H	-3.313090	2.799387	-2.070280
C	0.243386	6.069860	0.041240	H	0.687534	-7.011569	-0.258371	H	-5.755751	2.576892	-2.355905
C	0.933918	4.892451	0.174330	H	-1.787377	-6.949844	-0.445500	H	-7.178105	1.956190	-0.427223
C	2.408039	-2.443387	0.287866	H	-2.988084	-4.820137	-0.276537	H	-6.145919	1.577691	1.790055
C	-3.381259	-2.285201	0.050165	H	1.948232	-4.939097	0.077556	H	-3.706301	1.817100	2.075337
C	-3.343114	2.322479	0.020915	H	-2.810001	0.014324	0.294609				

(**2**)Ag^+

C	0.106291	6.027456	0.341106	C	2.902185	2.928181	-1.477308	H	1.897067	4.940770	0.064061
C	-1.303679	5.984337	0.509461	C	4.270035	3.061795	-1.699496	H	-3.024418	-4.753073	-0.623989
C	-1.956078	4.793488	0.476179	C	5.179891	2.773740	-0.690544	H	-1.851017	-6.901701	-0.678183
C	-1.253598	3.563855	0.268612	C	-4.159437	2.864479	-0.764744	H	0.616347	-6.981314	-0.372495
C	0.190687	3.603352	0.131327	C	-5.541770	2.734904	-0.782021	H	1.897018	-4.940793	-0.064051
C	0.823664	4.884367	0.164720	C	-6.183325	1.988307	0.198349	H	5.412717	2.178271	1.365716
C	-1.925461	2.343831	0.211715	C	-5.436278	1.365628	1.191829	H	2.973585	2.056192	1.796094
C	-1.160689	1.148990	0.096069	C	-4.055868	1.482866	1.202321	H	2.200896	3.148170	-2.271181
C	0.288472	1.172536	0.034386	C	-3.400294	2.239831	0.227807	H	4.623655	3.388931	-2.668159
C	0.943028	2.426136	-0.004733	C	-4.055884	-1.482845	-1.202330	H	6.241903	2.875801	-0.866488
N	-1.815605	0.000006	-0.000002	C	-5.436293	-1.365592	-1.191839	H	-3.661096	3.437290	-1.536014
C	-1.160701	-1.148985	-0.096071	C	-6.183346	-1.988250	-0.198350	H	-6.115976	3.215873	-1.562934
C	0.288459	-1.172546	-0.034387	C	-5.541797	-2.734842	0.782029	H	-7.260623	1.888393	0.186316
N	0.956064	-0.000008	-0.000001	C	-4.159467	-2.864432	0.764752	H	-5.929325	0.775761	1.952575
C	-1.925485	-2.343819	-0.211715	C	-3.400318	-2.239805	-0.227807	H	-3.478789	0.985215	1.968617
C	-1.253634	-3.563850	-0.268609	C	4.270006	-3.061818	1.699503	H	-3.478801	-0.985209	-1.968633
C	0.190651	-3.603360	-0.131323	C	2.902156	-2.928207	1.477311	H	-5.929335	-0.775730	-1.952592
C	0.943003	-2.426152	0.004734	C	2.409268	-2.531035	0.232787	H	-7.260642	-1.888324	-0.186317
C	-1.956124	-4.793477	-0.476178	C	3.337439	-2.256302	-0.795303	H	-6.116008	-3.215794	1.562949
C	-1.303735	-5.984331	-0.509457	C	4.717188	-2.365914	-0.558525	H	-3.661131	-3.437237	1.536029
C	0.106233	-6.027464	-0.341098	C	5.179864	-2.773761	0.690553	H	4.623625	-3.388953	2.668167
C	0.823616	-4.884381	-0.164713	Ag	3.302766	-0.000013	-0.000008	H	2.200866	-3.148196	2.271183
C	4.717213	2.365890	0.558532	H	0.616414	6.981301	0.372504	H	2.973561	-2.056224	-1.796091
C	3.337464	2.256273	0.795307	H	-1.850952	6.901712	0.678187	H	5.412694	-2.178297	-1.365708
C	2.409295	2.531008	-0.232784	H	-3.024372	4.753093	0.623987	H	6.241876	-2.875819	0.866500

($\underline{\mathbf{1}}$)$_2$Ag$^+$

Ag	-0.897236	1.628284	-0.672548	C	2.190219	2.923363	-1.627595	C	6.322591	-1.014846	1.542084
N	-1.999262	-1.626689	1.073758	C	2.321867	-2.504478	3.206517	C	-0.791615	-6.290746	1.746099
N	3.102184	-0.568000	-0.978573	C	5.494710	3.591911	-0.015203	C	7.529303	-1.050459	0.855279
N	-1.695071	1.043694	1.413188	C	3.427642	-2.031764	3.864901	C	-0.593407	-5.735187	3.005758
N	0.973155	0.862589	-1.983503	C	5.533848	4.963148	-0.051174	C	7.708513	-0.246727	-0.265080
C	-7.778435	1.092946	0.547072	C	3.556654	-0.658956	4.137818	C	-0.286925	-4.387605	3.134856
C	-1.113961	-4.695433	-3.490862	C	4.486449	5.691361	-0.644827	C	6.683637	0.582825	-0.701119
C	-7.893409	-0.275947	0.242974	C	2.595205	0.219488	3.706682	C	-0.166010	-3.572859	2.005003
C	0.020676	-5.409707	-3.065527	C	3.406578	5.030856	-1.174429	C	5.466283	0.625366	-0.017562
C	-6.790447	-1.089498	0.285804	C	-3.614471	4.632147	3.071106	C	-0.009625	4.328263	3.458966
C	1.086248	-4.752715	-2.504073	C	-2.382454	1.228137	-4.473388	C	-0.498249	4.274363	-3.928455
C	-5.517191	-0.574447	0.626943	C	-3.745731	3.273502	2.812719	C	-0.197239	2.952178	3.410120
C	1.074752	-3.347285	-2.339918	C	-1.305515	0.382421	-4.224412	C	0.695038	3.712266	-3.486255
C	-5.397991	0.819068	0.924823	C	-3.949498	2.812724	1.510562	C	0.647302	2.145129	2.644373
C	-0.065872	-2.620568	-2.805374	C	-1.263818	-0.383918	-3.060134	C	0.978804	3.626923	-2.123478
C	-6.559581	1.625121	0.883383	C	-4.015509	3.741252	0.470223	C	1.692310	2.747512	1.936832
C	-1.150458	-3.329489	-3.368502	C	-2.331037	-0.296381	-2.155974	C	0.042050	4.126722	-1.203944
C	-4.369606	-1.410015	0.697662	C	-3.893115	5.100283	0.730663	C	1.892687	4.119587	2.002509
C	2.152749	-2.654666	-1.720480	C	-3.405840	0.555823	-2.402358	C	-1.155236	4.683602	-1.653423
C	-3.153729	-0.860348	1.046232	C	-3.688313	5.549001	2.030381	C	1.036542	4.914169	2.757481
C	2.104267	-1.276584	-1.617583	C	-3.426207	1.325719	-3.561448	C	-1.429763	4.749645	-3.014600
C	-3.027344	0.527285	1.285141	C	-4.447004	-3.267939	-0.974454	H	-8.655797	1.725455	0.523646
C	0.998292	-0.557819	-2.131766	C	3.195876	-4.138998	0.009013	H	-1.950740	-5.223195	-3.928425
C	-4.117107	1.360479	1.247875	C	-4.401989	-4.617705	-1.298321	H	-8.859030	-0.689801	-0.015837
C	-0.078557	-1.202156	-2.689083	C	4.309056	-4.730178	0.591971	H	0.054570	-6.484838	-3.184727
C	-0.850382	-1.215444	1.734618	C	-4.317390	-5.573914	-0.293715	H	-6.883655	-2.143801	0.066916
C	3.217209	0.806766	-1.009700	C	5.569998	-4.548030	0.037468	H	1.952355	-5.308483	-2.174971
C	-0.683484	0.173514	1.953783	C	-4.281731	-5.176198	1.036936	H	-6.479241	2.674826	1.126997
C	2.149230	1.552758	-1.562259	C	5.712457	-3.779344	-1.111245	H	-2.013705	-2.776981	-3.713233
C	0.105195	-2.119864	2.156622	C	-4.328658	-3.826500	1.361794	H	2.228006	-3.560864	3.006079
C	4.341952	1.452849	-0.526550	C	4.598726	-3.193825	-1.698808	H	6.302365	3.040779	0.444379
C	1.287915	-1.633626	2.785979	C	-4.411647	-2.857608	0.359387	H	4.200532	-2.720121	4.180792
C	4.403502	2.875640	-0.563103	C	3.327140	-3.361459	-1.142754	H	6.376815	5.488295	0.378084
C	1.451038	-0.231086	3.007657	C	-0.368766	-4.143838	0.746105	H	4.420362	-0.292266	4.676110
C	3.327191	3.620748	-1.136473	C	5.299814	-0.180846	1.110662	H	4.532766	6.771594	-0.680788
C	0.445740	0.677202	2.553217	C	-0.680693	-5.491171	0.616902	H	2.704930	1.274877	3.908380

H	2.596757	5.589130	-1.624065
H	-3.471434	4.974730	4.087468
H	-2.404609	1.812130	-5.383733
H	-3.719535	2.559993	3.626839
H	-0.495443	0.308924	-4.939662
H	-4.183840	3.392420	-0.540627
H	-2.321117	-0.927436	-1.280213
H	-3.971481	5.813894	-0.079610
H	-4.224410	0.600697	-1.696321
H	-3.599848	6.608276	2.231439
H	-4.259710	1.986484	-3.758744
H	-4.503645	-2.523166	-1.757634
H	2.218550	-4.272923	0.449842
H	-4.427857	-4.921799	-2.336309
H	4.190498	-5.329438	1.485511
H	-4.277020	-6.625080	-0.546856
H	6.437512	-5.002838	0.497108
H	-4.210770	-5.915033	1.823604
H	6.690317	-3.632267	-1.549632
H	-4.297590	-3.516228	2.398633
H	4.711867	-2.596160	-2.594643
H	-0.271819	-3.532852	-0.139680
H	4.365237	-0.155615	1.653226
H	-0.833822	-5.905855	-0.368985
H	6.170101	-1.638209	2.412746
H	-1.035213	-7.340458	1.647974
H	8.326229	-1.702007	1.188632
H	-0.683372	-6.351299	3.890969
H	8.646082	-0.270152	-0.805112
H	-0.144972	-3.956126	4.116967
H	6.820416	1.198480	-1.580771
H	-0.673091	4.939118	4.055583
H	-0.698239	4.340357	-4.989690
H	-0.987604	2.495430	3.992836
H	1.420614	3.344025	-4.200993
H	2.356204	2.133803	1.344086
H	0.285144	4.134181	-0.148398
H	2.712250	4.567274	1.458396
H	-1.857731	5.074267	-0.932565
H	1.191275	5.983919	2.805650
H	-2.358572	5.182737	-3.360830
H	-2.128107	-2.623482	0.981633
H	3.884698	-1.091751	-0.618685
H	-1.692661	1.946395	1.876090
H	0.568817	1.302186	-2.802438

(**1**)(**2**)Ag^+

Ag	-0.946913	-1.973671	0.772318	C	2.270389	-2.926240	1.255143	C	6.455753	1.531133	-1.144872
N	-2.017268	1.688979	-0.946172	C	2.402781	2.655688	-2.807893	C	-0.822818	6.389371	-1.549155
N	3.174125	0.630798	1.044618	C	5.684135	-3.302029	-0.267193	C	7.692710	1.368243	-0.531546
N	-1.640313	-0.989174	-1.268439	C	3.515376	2.224132	-3.481603	C	-0.490514	5.834054	-2.780369
N	0.985169	-0.954112	1.661369	C	5.785004	-4.656631	-0.315759	C	7.876917	0.341190	0.386724
C	-7.754843	-1.135263	-0.615462	C	3.640374	0.872621	-3.845779	C	-0.166136	4.488196	-2.876695
C	-1.288144	4.319981	3.642392	C	4.754752	-5.472888	0.226700	C	6.832331	-0.525034	0.680440
C	-7.924793	0.251882	-0.455674	C	2.672036	-0.028089	-3.483025	C	-0.160426	3.670059	-1.741791
C	-0.152942	5.112617	3.323638	C	3.633227	-4.912544	0.754215	C	5.586652	-0.369654	0.065534
C	-6.842068	1.091772	-0.509691	C	-3.410113	-4.832887	-2.423974	C	-0.045419	-4.045547	-3.736057
C	0.925778	4.543475	2.728135	C	-2.549962	-1.810354	3.610055	C	-0.115248	-4.689560	3.595325
C	-5.535963	0.587010	-0.716532	C	-3.551149	-3.451446	-2.366863	C	-0.215581	-2.690763	-3.479625
C	0.946424	3.153944	2.382776	C	-1.403987	-1.050619	3.392301	C	0.932593	-3.912315	3.120924
C	-5.362733	-0.822189	-0.876085	C	-3.843240	-2.817431	-1.158936	C	0.674807	-2.003130	-2.650447
C	-0.219158	2.340988	2.699656	C	-1.461591	0.145250	2.653081	C	1.144225	-3.760768	1.748919
C	-6.503374	-1.656862	-0.825191	C	-3.977194	-3.593800	-0.004286	C	1.749038	-2.704506	-2.099334
C	-1.312720	2.991326	3.354417	C	-2.706867	0.539532	2.146938	C	0.273061	-4.402163	0.856243
C	-4.402654	1.442374	-0.768944	C	-3.856793	-4.975080	-0.066707	C	1.928672	-4.054516	-2.365055
C	2.067074	2.587635	1.775722	C	-3.849189	-0.216490	2.369226	C	-0.780966	-5.179433	1.339212
C	-3.152950	0.899241	-0.988317	C	-3.571725	-5.598526	-1.276245	C	1.026496	-4.731448	-3.178607
C	2.082654	1.182137	1.565044	C	-3.776095	-1.394513	3.102028	C	-0.978257	-5.321393	2.705708
C	-2.982421	-0.493940	-1.157677	C	-4.747528	3.412579	0.740622	H	-8.614802	-1.790905	-0.583839
C	0.923347	0.369399	1.877873	C	3.056675	4.392511	0.373713	H	-2.131101	4.774525	4.146198
C	-4.052915	-1.349668	-1.087281	C	-4.770600	4.782785	0.968195	H	-8.915480	0.658306	-0.300483
C	-0.249990	0.968417	2.402768	C	4.145827	5.114637	-0.094771	H	-0.140830	6.162488	3.584107
C	-0.815931	1.294205	-1.509200	C	-4.547085	5.668065	-0.079257	H	-6.977731	2.158436	-0.401510
C	3.259235	-0.688781	0.908067	C	5.419629	4.851045	0.393347	H	1.803622	5.133558	2.515234
C	-0.626464	-0.090135	-1.748857	C	-4.305065	5.177886	-1.356503	H	-6.382281	-2.721604	-0.962936
C	2.143525	-1.524884	1.283280	C	5.599055	3.858271	1.349918	H	-2.167926	2.403267	3.645886
C	0.145479	2.220997	-1.870313	C	-4.284023	3.808237	-1.584222	H	2.314120	3.695048	-2.532385
C	4.462250	-1.264186	0.408873	C	4.514740	3.126985	1.808482	H	6.465560	-2.684579	-0.682950
C	1.356412	1.764386	-2.466957	C	-4.503516	2.907995	-0.538311	H	4.298318	2.926970	-3.734020
C	4.545628	-2.657413	0.313755	C	3.228819	3.387914	1.329334	H	6.650946	-5.120483	-0.768500
C	1.520668	0.376969	-2.766007	C	-0.506093	4.241172	-0.514504	H	4.509635	0.538205	-4.395715
C	3.458485	-3.494632	0.791164	C	5.408426	0.677151	-0.841625	H	4.861522	-6.549560	0.205086
C	0.504635	-0.554101	-2.380317	C	-0.833438	5.587006	-0.416797	H	2.783075	-1.065845	-3.758236

H	2.846258	-5.540087	1.146302
H	-3.198097	-5.313390	-3.369668
H	-2.478110	-2.723665	4.184764
H	-3.472767	-2.860495	-3.270615
H	-0.462823	-1.372773	3.810961
H	-4.210684	-3.107340	0.933029
H	-2.767746	1.443336	1.563175
H	-3.991297	-5.565585	0.830124
H	-4.792882	0.105459	1.951744
H	-3.485481	-6.676003	-1.326437
H	-4.667195	-1.982556	3.277828
H	-4.921691	2.726629	1.559336
H	2.068667	4.594424	-0.015225
H	-4.963261	5.158327	1.964742
H	3.996803	5.883259	-0.842141
H	-4.562070	6.735180	0.098744
H	6.268779	5.415177	0.030330
H	-4.127260	5.860529	-2.176283
H	6.588522	3.641402	1.728982
H	-4.094998	3.427421	-2.579965
H	4.663709	2.344625	2.538468
H	-0.510706	3.628371	0.373361
H	4.447836	0.819513	-1.308652
H	-1.095340	6.000557	0.547067
H	6.298564	2.336722	-1.849274
H	-1.078074	7.438335	-1.476818
H	8.507556	2.042037	-0.762121
H	-0.488507	6.449889	-3.670331
H	8.833052	0.214729	0.877419
H	0.082588	4.060574	-3.838725
H	6.975083	-1.315389	1.405798
H	-0.739307	-4.559931	-4.387139
H	-0.256029	-4.805864	4.662097
H	-1.023867	-2.149679	-3.956346
H	1.603425	-3.421979	3.814084
H	2.455554	-2.178849	-1.475787
H	0.458601	-4.341841	-0.208046
H	2.770495	-4.577061	-1.931776
H	-1.432993	-5.675212	0.636702
H	1.166026	-5.783863	-3.387141
H	-1.791914	-5.930164	3.077108
H	-2.174851	2.683574	-0.889244
H	-1.619776	-1.862751	-1.782412

($\underline{\mathbf{2}}$)$_2$Ag$^+$

Ag	-0.220796	-2.547412	0.053467	C	2.982051	-2.414740	0.995239	C	5.656019	3.404910	-0.493698
N	-2.450287	1.496296	-1.240532	C	1.688243	3.648488	-2.490464	C	-2.477650	6.345251	-1.454281
N	2.634346	1.240846	1.118301	C	6.462295	-1.468777	-0.069153	C	6.791190	3.589437	0.287335
N	-1.259207	-1.004790	-1.441635	C	2.896226	3.571179	-3.103540	C	-1.794706	6.035014	-2.624287
N	1.065629	-1.035556	1.379859	C	7.022004	-2.699191	-0.207474	C	7.197206	2.586616	1.159431
C	-6.874014	-2.945017	-0.224830	C	3.371097	2.317825	-3.572997	C	-1.130252	4.821824	-2.742665
C	-2.961913	3.005729	3.510884	C	6.279780	-3.865253	0.126366	C	6.477949	1.401473	1.240786
C	-7.459220	-1.660367	-0.048824	C	2.680099	1.175374	-3.315747	C	-1.140528	3.894492	-1.695164
C	-2.163556	4.158943	3.296583	C	4.987433	-3.769689	0.538560	C	5.338488	1.205981	0.455589
C	-6.708820	-0.538389	-0.202716	C	-2.013234	-5.170087	-2.668780	C	1.242123	-3.508786	-3.627486
C	-0.928147	4.031020	2.750670	C	-1.805643	-3.035558	3.662736	C	1.230484	-5.178703	2.877370
C	-5.316972	-0.611725	-0.529501	C	-2.500879	-3.885061	-2.482222	C	0.646685	-2.306726	-3.274531
C	-0.414454	2.758513	2.339830	C	-1.031063	-1.956795	3.261970	C	1.885345	-3.989175	2.595026
C	-4.719842	-1.924370	-0.708355	C	-2.751229	-3.399382	-1.196923	C	1.358652	-1.330425	-2.564328
C	-1.241212	1.575636	2.533006	C	-1.576052	-0.922880	2.487044	C	2.187290	-3.638085	1.276663
C	-5.560095	-3.070429	-0.551484	C	-2.472885	-4.221226	-0.097613	C	2.676852	-1.622014	-2.197316
C	-2.511669	1.771383	3.161498	C	-2.914949	-1.037424	2.100121	C	1.787816	-4.493630	0.241419
C	-4.548934	0.540042	-0.703081	C	-1.991925	-5.514658	-0.291364	C	3.278937	-2.817196	-2.562221
C	0.880315	2.645600	1.832850	C	-3.696295	-2.106759	2.514050	C	1.137708	-5.691644	0.531935
C	-3.184381	0.401786	-1.072389	C	-1.764516	-5.991592	-1.573693	C	2.565193	-3.765180	-3.284782
C	1.378313	1.347553	1.538370	C	-3.147275	-3.108059	3.304893	C	0.861790	-6.037518	1.846396
C	-2.577331	-0.902911	-1.189166	C	-5.494674	2.288244	0.799515	H	-7.487868	-3.828810	-0.110459
C	0.546427	0.168561	1.689177	C	1.422141	4.853763	0.786888	H	-3.928872	3.107225	3.985680
C	-3.363137	-2.058158	-1.012768	C	-5.960986	3.575314	1.032607	H	-8.511233	-1.581652	0.190273
C	-0.774231	0.291552	2.185803	C	2.280394	5.926508	0.584614	H	-2.527570	5.130876	3.601251
C	-1.174931	1.398410	-1.597229	C	-6.033121	4.488936	-0.011327	H	-7.158999	0.436933	-0.096047
C	3.179568	0.044559	0.936292	C	3.502405	5.976944	1.242702	H	-0.299423	4.898155	2.625868
C	-0.551971	0.097328	-1.755832	C	-5.626991	4.112470	-1.286495	H	-5.131169	-4.050496	-0.697325
C	2.380644	-1.147508	1.111405	C	3.861694	4.946417	2.104015	H	-3.120537	0.912036	3.385000
C	-0.444112	2.597350	-1.833966	C	-5.149086	2.831618	-1.516627	H	1.317902	4.600360	-2.147733
C	4.553422	-0.041507	0.573149	C	3.011073	3.869921	2.297002	H	7.026115	-0.584336	-0.323394
C	0.873285	2.488019	-2.284856	C	-5.085856	1.901995	-0.477673	H	3.492235	4.462120	-3.247878
C	5.117374	-1.307442	0.394587	C	1.777613	3.809085	1.641907	H	8.036064	-2.796980	-0.571047
C	1.440262	1.185998	-2.600065	C	-1.859464	4.208650	-0.537458	H	4.302045	2.269825	-4.122157
C	4.334761	-2.503020	0.655055	C	4.930836	2.228378	-0.403847	H	6.747629	-4.837144	0.039436
C	0.761865	-0.003553	-2.273943	C	-2.507563	5.425485	-0.412350	H	3.066380	0.234557	-3.671702

H	4.429290	-4.663319	0.773934
H	-1.842476	-5.539030	-3.671648
H	-1.362502	-3.812876	4.270631
H	-2.716197	-3.255507	-3.335281
H	0.000730	-1.897624	3.571780
H	-2.700900	-3.872214	0.899959
H	-3.354489	-0.268443	1.484302
H	-1.805606	-6.143544	0.567223
H	-4.731758	-2.162050	2.206674
H	-1.403707	-7.000558	-1.724205
H	-3.756498	-3.939951	3.633001
H	-5.431933	1.580278	1.615474
H	0.474956	4.821494	0.269754
H	-6.269065	3.863004	2.029435
H	1.989395	6.723612	-0.087504
H	-6.400296	5.490944	0.167866
H	4.170839	6.813706	1.087474
H	-5.669131	4.822600	-2.101322
H	4.813710	4.973167	2.616521
H	-4.816871	2.548088	-2.505526
H	3.304279	3.067383	2.958038
H	-1.906683	3.497163	0.268851
H	4.041500	2.099725	-0.998101
H	-3.048893	5.646023	0.497329
H	5.321564	4.187471	-1.161245
H	-2.991634	7.292895	-1.360140
H	7.351747	4.512862	0.223494
H	-1.781382	6.735638	-3.448860
H	8.072669	2.726446	1.779911
H	-0.614726	4.580905	-3.662443
H	6.790054	0.627683	1.930002
H	0.674191	-4.241206	-4.185232
H	1.021814	-5.445852	3.905056
H	-0.372450	-2.110340	-3.568485
H	2.193383	-3.333539	3.398582
H	3.242473	-0.895299	-1.634824
H	2.048944	-4.253133	-0.779932
H	4.302170	-3.010465	-2.270299
H	0.858171	-6.350778	-0.277164
H	3.033714	-4.696639	-3.574313
H	0.369442	-6.974384	2.071613