

Supporting information for:

**Understanding the Interplay between π - π and
Cation- π Interactions in [Janusene-Ag]⁺
Host-Guest Systems: A computational Approach.**

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1 Quadrupole Moments

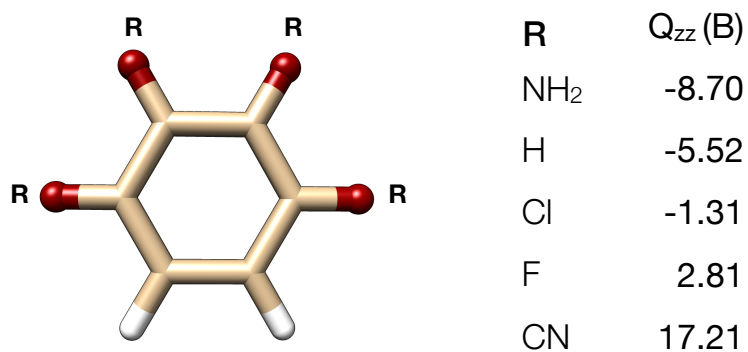


Figure S1: Quadrupole moments (Q_{zz}) of selected substituted aromatic rings, calculated at BP86-D3(BJ)/TZ2P level of theory. Color-code: white = hydrogens, tan = carbons, blue = nitrogen, red = oxygen.

2 Optimized Structures

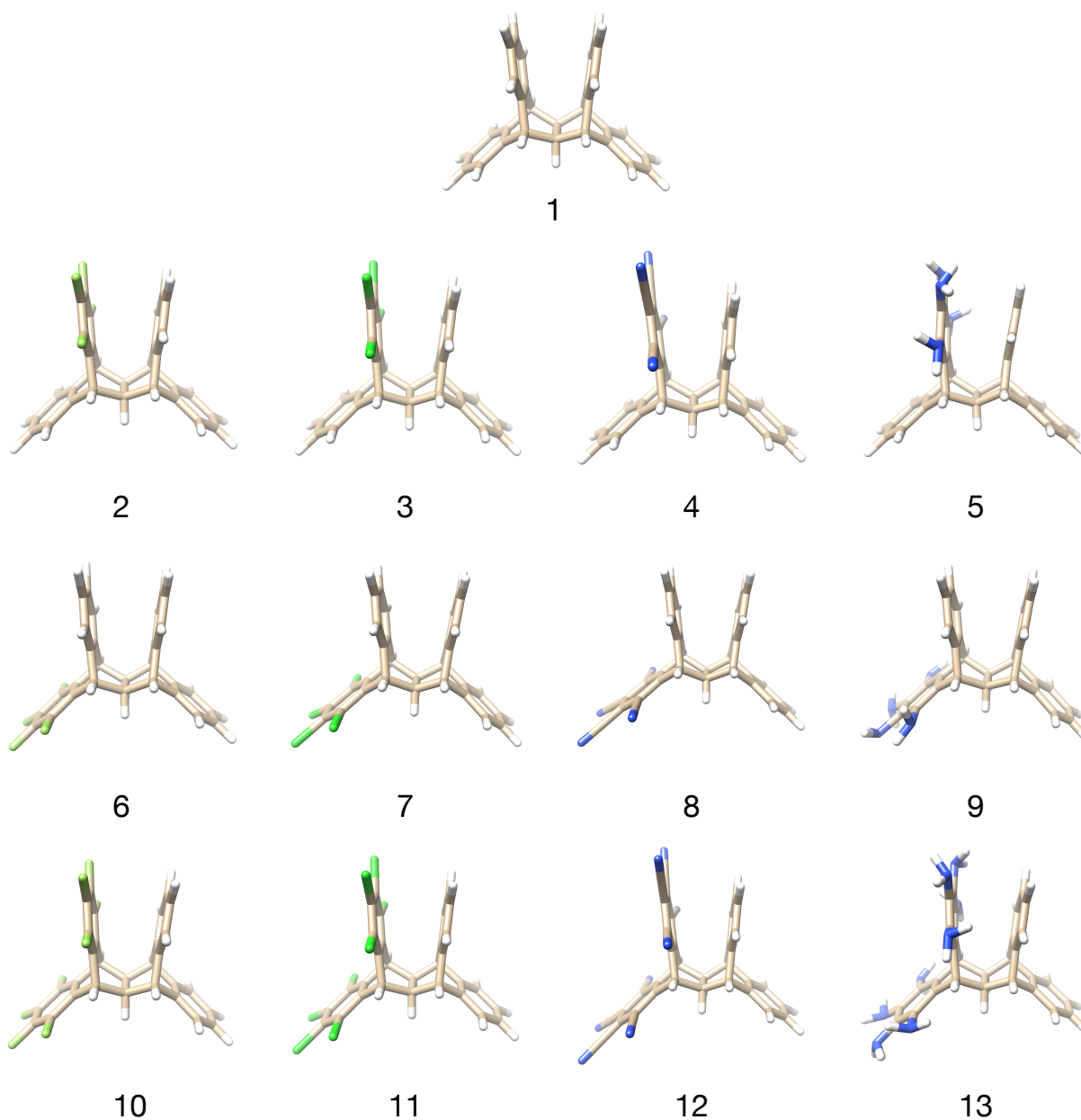


Figure S2: Compounds **1–13** optimized at PB86-D3(BJ)/Def2-TZVP level of theory. First row contains the **F** analogues (**2–5**), second row the **L** analogues (**6–9**), and third row **FL** analogues (**10–13**). Color-code: white = hydrogens, tan = carbons, blue = nitrogen, red = oxygen.

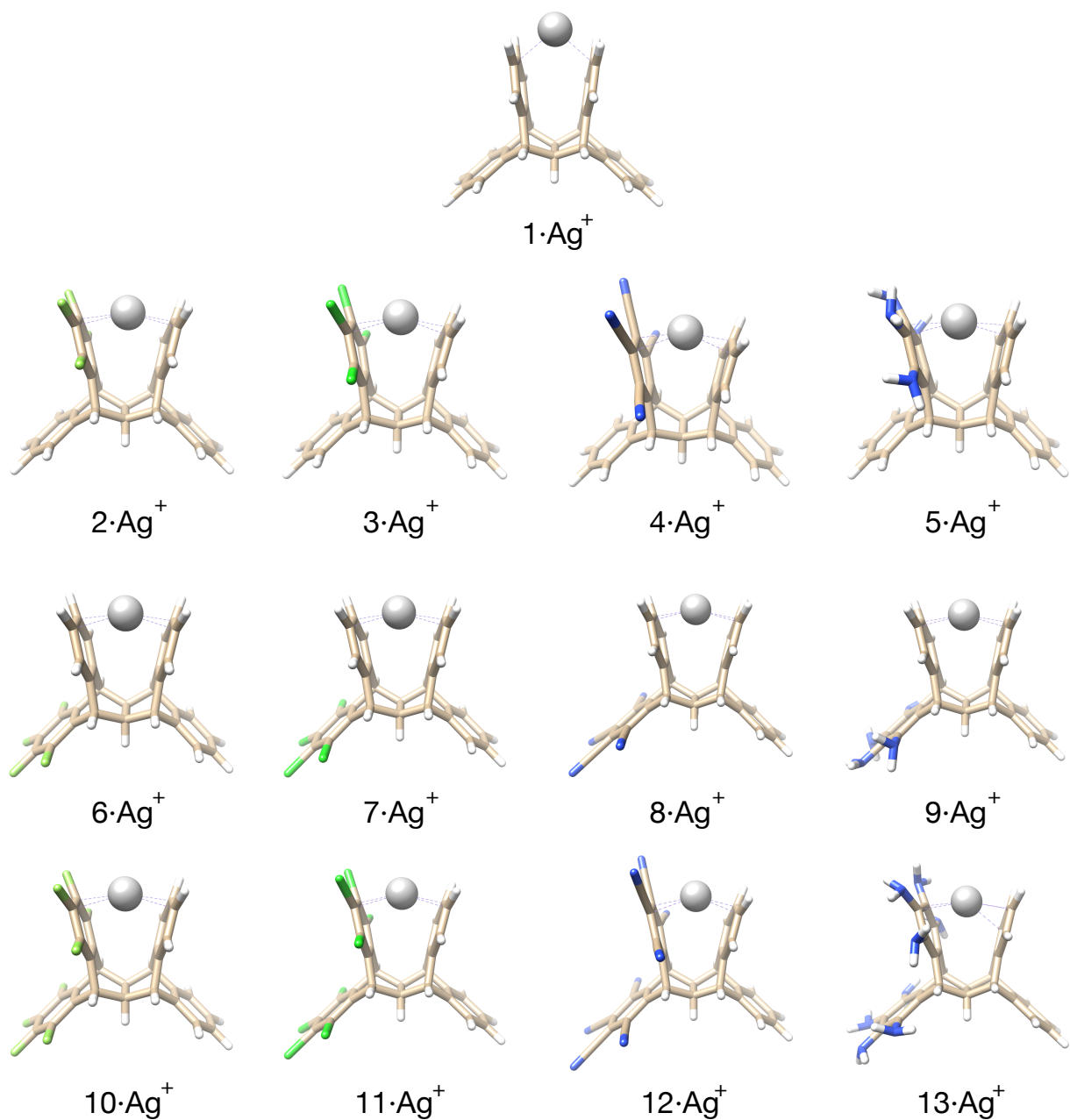


Figure S3: Complexes $1\cdot\text{Ag}^+$ – $13\cdot\text{Ag}^+$ optimized at PB86-D3(BJ)/Def2-TZVP level of theory. First row contains the **F** analogues ($2\cdot\text{Ag}^+$ – $5\cdot\text{Ag}^+$), second row the **L** analogues ($6\cdot\text{Ag}^+$ – $9\cdot\text{Ag}^+$), and third row **FL** analogues ($10\cdot\text{Ag}^+$ – $13\cdot\text{Ag}^+$). Color-code: white = hydrogens, tan = carbons, blue = nitrogen, red = oxygen. Color-code: white = hydrogens, tan = carbons, blue = nitrogen, red = oxygen.

Table S1: Natural charge in substituted janusenes and in it complexes

	NPA charges						
	Janusene		[Ag(Janusene)] ⁺				Ag
	C2/C3	C2'/C3'	C2	C3	C2'	C3'	
1	-0.214	-0.214	-0.370	-0.237	-0.370	-0.239	0.795
2	0.258	-0.217	0.146	0.256	-0.366	-0.241	0.768
3	-0.099	-0.218	-0.256	-0.134	-0.375	-0.251	0.848
4	-0.079	-0.216	-0.215	-0.093	-0.387	-0.235	0.866
5	0.096	-0.225	0.058	0.006	-0.360	-0.229	0.756
6	-0.210	-0.213	-0.358	-0.250	-0.371	-0.236	0.799
7	-0.210	-0.213	-0.368	-0.234	-0.368	-0.240	0.798
8	-0.202	-0.211	-0.364	-0.228	-0.368	-0.236	0.804
9	-0.216	-0.214	-0.344	-0.283	-0.376	-0.229	0.792
10	0.261	-0.216	0.148	0.258	-0.366	-0.240	0.772
11	-0.097	-0.217	-0.256	-0.130	-0.377	-0.247	0.849
12	-0.071	-0.213	-0.204	-0.085	-0.389	-0.231	0.873
13	0.096	-0.221	0.062	0.002	-0.363	-0.226	0.750

3 Natural Charges

4 XYZ Cartesian Coordinates

1 E=-1157.784368155155 Hartree

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C	0.48674967154040	-1.63746059998755	-1.39955561574136
C	0.75848302384380	-1.76431466732667	1.17971872101336
C	0.59819814881409	0.89015969887751	1.30071652367246
C	0.42687065331910	1.02432722022631	-1.28706206016233
C	1.60791507679148	-2.78548055448637	0.44190844799218
C	2.48097531542789	-3.70836846174851	1.00952621744788
C	3.19983760912219	-4.58015634276838	0.17959620938190
C	3.04755060181963	-4.51800317160829	-1.20707591978445
C	2.17491317352751	-3.58207494963231	-1.78057189844786
C	1.45551309081724	-2.72155924645880	-0.95733346300433
C	-0.66464181015850	-1.98910350192735	0.72137236329518
C	-1.75905630324138	-2.28383536957031	1.52786442994152
C	-3.01151280510764	-2.49655382935854	0.94049009596293
C	-3.16095820506415	-2.41186530079728	-0.44528923103894
C	-2.05920967443433	-2.11828568012843	-1.25705737587292
C	-0.81294930599815	-1.91060726888377	-0.67439734518115
C	-0.82301132733559	1.04000682231542	0.80253115010900

C	-1.96974094941745	1.13708780229624	1.58418043806548
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C	1.29149415180130	2.12228607069745	-0.69060397098069
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C	2.82326748892567	3.98722239102224	0.71279430673958
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C	1.97181837868830	3.11704590963831	-1.38645384712125
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H	2.05565373592220	-3.53093444623319	-2.86540925082890
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H	0.35813778703255	-1.61410774292217	-2.49087284710459
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Cl	-4.69978802477373	-2.32874835262829	-1.22509422324184
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H	-4.28242142878779	1.37969572677389	-0.83537229373868
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4 E=-1527.223775999567 Hartree

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C	1.67883412561887	-4.38648133803393	-0.61662493827678
C	0.72377884817040	-3.75525410254712	0.17445772286984
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5 E=-1379.546233849951 Hartree

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6 E=-1555.489905442042 Hartree

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7 E=-3005.490298446442 Hartree

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9 E=-1379.534921842688 Hartree

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H	2.32436220338193	-0.36177730249218	0.95462346572695
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H	3.85621883354340	-5.34940391894934	0.74704866290286
H	2.58888481084882	3.63063652232379	-3.34270303877312
H	0.97834947990343	3.17438936608564	-3.28812550332717
H	2.85546621784647	5.38261765817057	-2.25616505310332

H	3.66698666245491	5.75406559935943	-0.83597809907636
H	4.66092121438261	4.79446619563738	1.20531235748666
H	3.36427438300180	5.05529078242614	2.21598060269173
H	3.33273954384717	2.95152011892508	3.05932377052778
H	-1.89133775187013	1.09881852260900	2.65971783615031
H	-2.23193007617312	1.27661289986012	-2.31577353795592
H	-4.27876779820370	1.52005401601747	-0.91045013273049
H	-4.10942722364018	1.42746518494383	1.56702733716914
H	1.88391586199435	2.15129259564995	3.20381460501466

10 E=-1953.189406650359 Hartree

C	1.15352785341669	-0.31685668826896	-0.88512111946983
C	0.52090069369743	-1.64984593459271	-1.41381252533947
C	0.77471963173852	-1.77842931788287	1.17749246940061
C	0.60667665405105	0.87099027072563	1.30540128176552
C	0.41557928673852	1.00374846434150	-1.28291620100282
C	1.62332227863307	-2.79933371317589	0.44040853074679
C	2.49445064619669	-3.71662010632157	1.00494480904697
C	3.23259704525745	-4.58507710495075	0.18891776449621
C	3.09353354535596	-4.51928183994491	-1.19914546977151
C	2.21701068160595	-3.58488950676998	-1.76800701468940
C	1.48334140093826	-2.73286096229564	-0.95884718933926
C	-0.64460998306846	-1.99026885711379	0.70246681009923
C	-1.75877435516576	-2.20111147468821	1.49591232421014
C	-3.02362862954003	-2.33762420578588	0.91457483143441
C	-3.16103950965046	-2.25905093466778	-0.47217428658580
C	-2.03258066607375	-2.04715328711769	-1.27149950181309
C	-0.78181694457856	-1.91433768807729	-0.69358359138375
C	-0.82044242175969	1.00396358661304	0.81784488984164
C	-1.96130032207060	1.09489865510619	1.61006262776638
C	-3.21185305537546	1.26343632556564	1.00157881770347
C	-3.31344344655798	1.34058895605672	-0.38948304188727
C	-2.16595476227297	1.24885093776715	-1.18727623862749
C	-0.92349147523854	1.08124840444147	-0.58278140804005
C	1.26977751583806	2.11295897477499	-0.69076134851288
C	1.37028420839057	2.04335454852044	0.71217130773404
C	2.13178746601425	2.97702538005172	1.40830007640009
C	2.78920764590778	3.99380429528196	0.70187092056977
C	2.68882407903373	4.06369913907472	-0.68925683996712
C	1.93013889271629	3.11724060460995	-1.39201540597013
F	2.65487553396536	-3.79615278266378	2.34449041954523
F	3.80010391867582	-5.35272162942993	-1.97983866628044
F	2.10831213462556	-3.53749753580652	-3.11413204417238

F	-1.65913824037687	-2.23644186850285	2.84409499885853
F	-4.11093605402472	-2.51415371065017	1.68281389895681
F	-4.37944220377618	-2.36124449607793	-1.02791981379338
F	-2.19864477120893	-1.93501800559509	-2.60868713465463
H	-1.88085366438239	1.03111322280273	2.69742625840510
H	-4.10902939448344	1.33424580551719	1.61739202409274
H	-4.28952723023560	1.47242934133481	-0.85746115851398
H	-2.24455269151517	1.30238664565697	-2.27521993247848
H	2.21109706422028	2.92077576953234	2.49636211086062
H	3.37906114519275	4.73500245776219	1.24288789465274
H	3.20040344669853	4.85942759131372	-1.23226257295853
H	2.15554010185160	-0.25950322100006	-1.33187131825310
H	0.32215138145950	1.08754401269191	-2.37440155296629
H	0.67312809470469	0.84168441503963	2.40190782258894
H	0.39954269365492	-1.63057825650244	-2.50185410256910
H	0.86858627097699	-1.86689439886654	2.26523315473334
C	1.28682340328079	-0.38783696842086	0.67113740495576
H	2.34954669862804	-0.33584329775443	0.94606434746598
H	1.85338794297814	3.16973250127167	-2.48052764035946
F	4.07160546491233	-5.48171951292974	0.73250932306858

11 E=-4853.203139665311 Hartree

C	1.16866220201341	-0.29958342135496	-0.88550212824376
C	0.54305826390183	-1.63517144542534	-1.41041762770964
C	0.78397232783871	-1.76269541336255	1.16417082592645
C	0.62277770151687	0.88164651192267	1.30849122420935
C	0.41594388956917	1.01441993978198	-1.27942924069144
C	1.63242321211311	-2.78917058161766	0.43769088306608
C	2.49296355511751	-3.71618803725210	1.01869443863550
C	3.22837215309109	-4.59880164751992	0.20056981856640
C	3.09592415660237	-4.53066729034615	-1.19956541671161
C	2.22916878702103	-3.57986800479765	-1.77711269841876
C	1.50100089157712	-2.72107999958089	-0.95859888110453
C	-0.63596040151954	-1.96788556030201	0.69023923209061
C	-1.75550357509360	-2.16565771608611	1.49173366103728
C	-3.02735789577893	-2.28426386718942	0.90107477915071
C	-3.15826737238921	-2.21312775871156	-0.49818735488818
C	-2.01649783303816	-2.02455955121918	-1.29935720523282
C	-0.76618964931447	-1.89657953643749	-0.70336926375962
C	-0.80843095109946	1.00410234624610	0.82961912875790
C	-1.94592475372549	1.07855605942840	1.62823583119332
C	-3.20294553662459	1.21792305338291	1.02628576297778
C	-3.31332890419034	1.29119384053935	-0.36420419344221

C	-2.16826477367881	1.22625373227855	-1.16771590469895
C	-0.91990556984397	1.07911853179779	-0.57052761371492
C	1.26522131365313	2.12929717104100	-0.69119847383884
C	1.37552385707586	2.05863592334853	0.71117166181573
C	2.13501920508602	2.99695920863129	1.40322596558719
C	2.78018131830768	4.01954695661052	0.69386651918671
C	2.66992261830220	4.09054712716264	-0.69645888898427
C	1.91364027976775	3.13926211639180	-1.39535992872578
C1	2.65780297165201	-3.78426072124840	2.74474312249682
C1	3.98982504000958	-5.61044005118222	-2.20356878430273
C1	2.06869484079891	-3.48005472059496	-3.50151689738517
C1	-1.59022872378559	-2.19495053583414	3.21681602152754
C1	-4.42661338238863	-2.46057569212525	1.89038218245638
C1	-4.71841038971673	-2.30249894722200	-1.22333044141806
C1	-2.17436661239624	-1.88595784096390	-3.02007787648368
H	-1.85880075175513	1.01556187868392	2.71485757430915
H	-4.09852318403582	1.26442243060114	1.64640832683012
H	-4.29463060731846	1.39605045570201	-0.82774502146437
H	-2.25408088282149	1.27646075467056	-2.25511438685336
H	2.22191792436890	2.93976859986925	2.49064634197974
H	3.36827651762865	4.76432909374402	1.23192990631327
H	3.17206767950641	4.89073591162393	-1.24175139583424
H	2.16803157683102	-0.23459857340984	-1.33731141021846
H	0.31415824363750	1.09620232555725	-2.37008218187424
H	0.69630636047535	0.84929290393592	2.40420813538896
H	0.42541984404002	-1.61727130451095	-2.49763374262380
H	0.87302303748996	-1.85413568502715	2.25043396854398
C	1.30365719172057	-0.37345045827733	0.66749714446908
H	2.36580286775887	-0.32735592882993	0.94585519502437
H	1.82920895664017	3.19236606501551	-2.48326289236969
C1	4.28504396540190	-5.75999564753797	0.91295719945269

12 E=-1896.637982752867 Hartree

C	0.36495700000000	-1.48449900000000	0.96509000000000
C	-0.03458400000000	-2.48853600000000	-0.17809400000000
C	-0.69432300000000	-3.49426400000000	2.13572900000000
C	-0.81287900000000	-1.06063200000000	3.19071600000000
C	-0.24737900000000	-0.04926200000000	0.86090700000000
C	0.34837400000000	-4.30855700000000	1.39945300000000
C	0.97968600000000	-5.46170100000000	1.88079900000000
C	1.98131700000000	-6.09136400000000	1.09424800000000
C	2.34077900000000	-5.54465700000000	-0.15628500000000
C	1.70096600000000	-4.36559600000000	-0.62399300000000

C	0.70766600000000	-3.76379000000000	0.15738600000000
C	-1.85649700000000	-3.35071800000000	1.18277800000000
C	-3.18932400000000	-3.67347000000000	1.46011300000000
C	-4.17938400000000	-3.47682200000000	0.46507700000000
C	-3.81672500000000	-2.95895600000000	-0.79584000000000
C	-2.46450100000000	-2.62566700000000	-1.05801000000000
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C	-2.03824400000000	-0.63701200000000	2.41294900000000
C	-3.35952600000000	-0.72182800000000	2.84281600000000
C	-4.38585200000000	-0.27766400000000	1.99895000000000
C	-4.08442500000000	0.25241100000000	0.74141000000000
C	-2.75313500000000	0.34847000000000	0.31427600000000
C	-1.73328500000000	-0.09822000000000	1.15017900000000
C	0.39701800000000	0.70512600000000	2.01239800000000
C	0.09584200000000	0.15464100000000	3.27175500000000
C	0.62287100000000	0.71758500000000	4.42969200000000
C	1.44975200000000	1.84430800000000	4.32820600000000
C	1.74876600000000	2.39052800000000	3.07810300000000
C	1.22588700000000	1.81801500000000	1.91108900000000
C	0.62734200000000	-5.98435500000000	3.15996500000000
C	3.34938000000000	-6.16778300000000	-0.94585100000000
C	2.07413100000000	-3.78492900000000	-1.87196000000000
C	-3.55008200000000	-4.12560300000000	2.76201300000000
C	-5.54515300000000	-3.74677300000000	0.76100700000000
C	-4.81393700000000	-2.71007600000000	-1.78029000000000
C	-2.09301100000000	-2.01709400000000	-2.29139100000000
H	-3.59457200000000	-1.13733100000000	3.82437400000000
H	-5.42384500000000	-0.34529900000000	2.32635200000000
H	-4.88756300000000	0.59579900000000	0.08906000000000
H	-2.51828600000000	0.76486200000000	-0.66702800000000
H	0.38758900000000	0.29112400000000	5.40658000000000
H	1.85748300000000	2.29863500000000	5.23143500000000
H	2.38903900000000	3.27049500000000	3.00842600000000
H	1.45426700000000	-1.36949500000000	0.88942600000000
H	-0.02257900000000	0.40252800000000	-0.11439900000000
H	-1.06043400000000	-1.46589800000000	4.18020400000000
H	0.23202600000000	-2.09592700000000	-1.16638500000000
H	-0.98535800000000	-3.95106100000000	3.08843500000000
C	0.00003300000000	-2.09963300000000	2.35264100000000
H	0.91982400000000	-2.31139600000000	2.91540700000000
H	1.45864100000000	2.24466100000000	0.93396600000000
C	2.62599500000000	-7.26799500000000	1.57250300000000
N	3.14811700000000	-8.22882400000000	1.97356500000000
N	0.31534700000000	-6.37340500000000	4.21278900000000
N	4.17394300000000	-6.66823000000000	-1.59878700000000

N	2.35460100000000	-3.27460900000000	-2.88094500000000
N	-3.80052900000000	-4.46695200000000	3.84731500000000
N	-6.66101100000000	-3.95862500000000	1.01931200000000
N	-5.62310400000000	-2.48902800000000	-2.58857800000000
N	-1.74601500000000	-1.49466100000000	-3.27327300000000

13 E=-1601.300489408853 Hartree

C	1.15482900000000	-0.16266600000000	-0.88100000000000
C	0.45229800000000	-1.45064800000000	-1.42550600000000
C	0.56072200000000	-1.55718000000000	1.16410400000000
C	0.76150600000000	1.09056800000000	1.29968900000000
C	0.48859300000000	1.20253900000000	-1.25187800000000
C	1.34772200000000	-2.67007600000000	0.49204800000000
C	2.09101600000000	-3.66446100000000	1.12046200000000
C	2.78052300000000	-4.60714600000000	0.34455900000000
C	2.73134300000000	-4.54255800000000	-1.04941800000000
C	1.99040300000000	-3.53511600000000	-1.68386500000000
C	1.29775300000000	-2.60504200000000	-0.91501500000000
C	-0.85035500000000	-1.65855300000000	0.61888700000000
C	-2.01342800000000	-1.86230400000000	1.35613200000000
C	-3.23383100000000	-2.03149100000000	0.69066100000000
C	-3.28778400000000	-2.00175300000000	-0.70474400000000
C	-2.11832900000000	-1.79730000000000	-1.44709300000000
C	-0.90650200000000	-1.61696900000000	-0.78557400000000
C	-0.67697000000000	1.30080300000000	0.88346100000000
C	-1.78995100000000	1.30753700000000	1.72394700000000
C	-3.07318500000000	1.36219500000000	1.14778300000000
C	-3.22080300000000	1.50022000000000	-0.23886200000000
C	-2.09443400000000	1.45650800000000	-1.08399400000000
C	-0.82672600000000	1.34880400000000	-0.51283000000000
C	1.44434800000000	2.25973000000000	-0.72356400000000
C	1.59543700000000	2.19605500000000	0.67395600000000
C	2.42528200000000	3.09864100000000	1.34216700000000
C	3.12390500000000	4.06588100000000	0.58840000000000
C	3.04971700000000	4.06403600000000	-0.81237100000000
C	2.17626100000000	3.17836400000000	-1.47880600000000
H	2.13200000000000	-3.71257200000000	2.21134400000000
H	3.26845700000000	-5.28001800000000	-1.64774700000000
H	1.95173300000000	-3.48302900000000	-2.77467100000000
H	-1.97458900000000	-1.87656300000000	2.44726700000000
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H	-4.24135500000000	-2.13659900000000	-1.21622100000000
H	-2.15051400000000	-1.78783700000000	-2.53987000000000

N	-1.72240800000000	1.12699900000000	3.13624100000000
N	-4.22365700000000	1.28172600000000	1.96125900000000
N	-4.51636700000000	1.55891400000000	-0.79405700000000
N	-2.34420500000000	1.50998900000000	-2.48533300000000
N	2.56420500000000	3.16490300000000	2.76138600000000
N	3.95709100000000	5.00321900000000	1.23910400000000
N	3.79851800000000	5.00703900000000	-1.55070900000000
H	2.16353500000000	-0.14996600000000	-1.31744500000000
H	0.36212500000000	1.25871700000000	-2.34405800000000
H	0.88700700000000	1.04148400000000	2.39258200000000
H	0.39620500000000	-1.43226300000000	-2.52366000000000
H	0.58749500000000	-1.63531000000000	2.26084000000000
C	1.27116000000000	-0.24808400000000	0.67364600000000
H	2.33065100000000	-0.34743000000000	0.95053900000000
N	2.14967700000000	3.24935800000000	-2.90386000000000
H	3.35523100000000	-5.39533500000000	0.83338100000000
H	-4.96239500000000	0.75018200000000	1.49472600000000
H	-3.99323600000000	0.82745800000000	2.84807600000000
H	-4.47841800000000	1.94603300000000	-1.73940400000000
H	-5.15093100000000	2.11602900000000	-0.21939700000000
H	-1.47939100000000	1.57050000000000	-3.01879300000000
H	-2.85016400000000	0.67517100000000	-2.79908100000000
H	-0.76475500000000	1.00386100000000	3.45853200000000
H	-2.13163700000000	1.91434000000000	3.64469100000000
H	1.77323100000000	4.14137300000000	-3.23463100000000
H	1.59490900000000	2.49975500000000	-3.31235200000000
H	3.91513700000000	4.68403100000000	-2.51407600000000
H	4.71649900000000	5.16731100000000	-1.13159300000000
H	3.92470600000000	5.91626800000000	0.78118300000000
H	3.67148700000000	5.10237700000000	2.21642700000000
H	3.50980600000000	2.92643400000000	3.06958800000000
H	1.90731300000000	2.55041800000000	3.23779700000000

1·Ag⁺ E=-6537.965087062790 Hartree

C	1.09276606440241	-0.29499452876853	-0.88012540893628
C	0.47130537906783	-1.63343248325558	-1.41075360807199
C	0.72012864521894	-1.75780481235963	1.18732330395240
C	0.58520915409291	0.91573928250174	1.31603856875931
C	0.38862058767216	1.04516609082513	-1.28636283735905
C	1.58644493219041	-2.78052389096738	0.45318047589254
C	2.46263766177378	-3.70259430575596	1.03785078653041
C	3.20470578996255	-4.56731418870193	0.20791537358783
C	3.06694364617774	-4.50449324401463	-1.18968853880014

C	2.18570612448988	-3.57453205873007	-1.77836187060112
C	1.44874619843744	-2.71604218941712	-0.95401124370227
C	-0.69204011323617	-2.02696430780784	0.71351920639422
C	-1.77367453830557	-2.41393590443478	1.51252126428419
C	-3.01338841638869	-2.76085049073774	0.90562744877519
C	-3.15361072142546	-2.68589377020584	-0.51563200356489
C	-2.04862730795120	-2.26534848673122	-1.31304336580953
C	-0.82869331167634	-1.95318196344913	-0.70256656704138
C	-0.83694554032642	1.11519045077463	0.83515399844641
C	-1.96203217758545	1.32263196603674	1.64099607092854
C	-3.21671032147139	1.63670998377663	1.04033085186123
C	-3.32040751677353	1.71418712392467	-0.38383409968775
C	-2.17199562227555	1.47435113049788	-1.18977371159717
C	-0.94329392412787	1.19098010126872	-0.58338745037560
C	1.27032877771218	2.14523623630125	-0.69625036614176
C	1.37402543124157	2.07743338551588	0.71360899342179
C	2.16039223635052	3.00170201734397	1.41169253665478
C	2.84475288249697	4.00341176405845	0.69359608396373
C	2.74081078256037	4.07176382014452	-0.70665913624030
C	1.95160398243017	3.13871306029427	-1.40966924827347
H	-1.66326956813745	-2.48936295138454	2.60237084436317
H	-3.82224609522455	-3.18876041403759	1.51369264668941
H	-4.06313530213546	-3.07016277310985	-0.99830978427624
H	-2.15202988313656	-2.22907158483828	-2.40610661136365
H	-1.87920132707994	1.28601495174995	2.73565759984089
H	-4.06451917990621	1.94134592509568	1.66946090044463
H	-4.25291790569804	2.06537676618543	-0.84672613982073
H	-2.25048049292943	1.55081845896291	-2.28250265551243
H	2.24335688312497	2.94787022832023	2.50647241970002
H	3.45947158715327	4.73561574638856	1.23342345120843
H	3.27438330300733	4.85731980673353	-1.25743014894073
H	2.10165592168410	-0.24297745762812	-1.32632875104397
H	0.29349529025508	1.12733186935138	-2.38393154848843
H	0.65397002958727	0.88707171173164	2.41853655516861
H	0.35427017004504	-1.60898876111766	-2.50889389399171
H	0.81489227763271	-1.83644910700925	2.28552481922884
C	1.22601336287676	-0.36491870348428	0.67843777606880
H	2.29594578216541	-0.32318792998408	0.95085786058255
H	1.87246193922582	3.19144093002201	-2.50489772759479
H	2.07838196910773	-3.52500022916208	-2.87125902140282
H	3.64667592008033	-5.18414429679090	-1.82775397143161
H	3.89187206524106	-5.29571121055947	0.65829326484794
H	2.57111070027860	-3.75194956414115	2.13052941069040
Ag	-3.67260821195204	-0.54583419922117	0.30167319778355

2·Ag⁺ E=-6935.644279693110 Hartree

C	1.11450500000000	-0.30198100000000	-0.88341300000000
C	0.49194300000000	-1.63759800000000	-1.41538400000000
C	0.74001400000000	-1.76220700000000	1.18432000000000
C	0.60968000000000	0.90673600000000	1.31513100000000
C	0.41034800000000	1.03751100000000	-1.28812300000000
C	1.59984500000000	-2.79062500000000	0.44983700000000
C	2.46981100000000	-3.71740500000000	1.03574700000000
C	3.20684400000000	-4.58646400000000	0.20558100000000
C	3.07051900000000	-4.52263300000000	-1.19208000000000
C	2.19544400000000	-3.58740700000000	-1.78200900000000
C	1.46331200000000	-2.72538900000000	-0.95751600000000
C	-0.67216100000000	-2.02508800000000	0.70580600000000
C	-1.73646600000000	-2.43720500000000	1.50586600000000
C	-2.97295200000000	-2.80620900000000	0.90242000000000
C	-3.12061000000000	-2.71843200000000	-0.52151700000000
C	-2.01209500000000	-2.29135800000000	-1.31840800000000
C	-0.80811400000000	-1.95221200000000	-0.70361500000000
C	-0.81276300000000	1.10503900000000	0.83607000000000
C	-1.93655400000000	1.31606600000000	1.64462600000000
C	-3.18899200000000	1.64181000000000	1.04570700000000
C	-3.29570100000000	1.71796900000000	-0.37977000000000
C	-2.14927000000000	1.46883800000000	-1.18899600000000
C	-0.92042900000000	1.18102100000000	-0.58316400000000
C	1.29048900000000	2.13888200000000	-0.69744200000000
C	1.39549200000000	2.07039800000000	0.71210200000000
C	2.17928400000000	2.99636900000000	1.41079300000000
C	2.86023300000000	4.00035800000000	0.69273500000000
C	2.75511900000000	4.06940500000000	-0.70744100000000
C	1.96809900000000	3.13485100000000	-1.41088300000000
H	2.57714300000000	-3.76765400000000	2.12839500000000
H	3.64640300000000	-5.20588200000000	-1.82969800000000
H	2.08904900000000	-3.53737500000000	-2.87487800000000
F	-1.62558600000000	-2.53077200000000	2.82685900000000
F	-3.93517900000000	-3.36533400000000	1.62439600000000
F	-4.20555900000000	-3.22935600000000	-1.09722500000000
F	-2.15940100000000	-2.26150400000000	-2.63848000000000
H	-1.85269400000000	1.27757100000000	2.73917500000000
H	-4.03711600000000	1.94384500000000	1.67540100000000
H	-4.22626800000000	2.07756500000000	-0.84034700000000
H	-2.22933700000000	1.54591600000000	-2.28161500000000
H	2.26297400000000	2.94209800000000	2.50544500000000
H	3.47312200000000	4.73396900000000	1.23266500000000
H	3.28597500000000	4.85696200000000	-1.25789800000000

H	2.12295800000000	-0.25177800000000	-1.33049900000000
H	0.31339500000000	1.12059900000000	-2.38533500000000
H	0.67981700000000	0.87722100000000	2.41735700000000
H	0.36866500000000	-1.61439000000000	-2.51116500000000
H	0.82632800000000	-1.84364000000000	2.28126000000000
C	1.24876500000000	-0.37271100000000	0.67560300000000
H	2.31879800000000	-0.33439100000000	0.94763800000000
H	1.88793600000000	3.18847900000000	-2.50594000000000
H	3.88897100000000	-5.31929900000000	0.65628500000000
Ag	-3.62364000000000	-0.52483400000000	0.25046600000000

3·Ag⁺ E=-8385.658488809720 Hartree

C	1.14986300000000	-0.31503000000000	-0.88592800000000
C	0.55051600000000	-1.65724000000000	-1.42319500000000
C	0.77809100000000	-1.78362900000000	1.17080700000000
C	0.63337700000000	0.87774800000000	1.31769300000000
C	0.41159900000000	1.00702700000000	-1.28432700000000
C	1.64145800000000	-2.81240800000000	0.44501700000000
C	2.50166800000000	-3.74424600000000	1.03786600000000
C	3.24316600000000	-4.61326900000000	0.21195600000000
C	3.11936800000000	-4.54624100000000	-1.18716600000000
C	2.25223100000000	-3.60795300000000	-1.78329300000000
C	1.51782600000000	-2.74409400000000	-0.96232500000000
C	-0.63459500000000	-2.03807400000000	0.68524100000000
C	-1.73456000000000	-2.37633900000000	1.48205900000000
C	-2.98204600000000	-2.71533500000000	0.86771700000000
C	-3.10655900000000	-2.64870100000000	-0.56462500000000
C	-1.98086100000000	-2.24294300000000	-1.35004800000000
C	-0.75783400000000	-1.97039500000000	-0.72657900000000
C	-0.79578800000000	1.06196200000000	0.85112400000000
C	-1.90788400000000	1.28899000000000	1.67059300000000
C	-3.16030600000000	1.63597400000000	1.08394400000000
C	-3.28174400000000	1.70597300000000	-0.34185200000000
C	-2.14913800000000	1.42812400000000	-1.16197600000000
C	-0.91674400000000	1.13221000000000	-0.56763800000000
C	1.27512800000000	2.12510800000000	-0.69919000000000
C	1.39532700000000	2.05507600000000	0.70932700000000
C	2.16826200000000	2.99412800000000	1.40245500000000
C	2.82275500000000	4.01278100000000	0.68036200000000
C	2.70210100000000	4.08350800000000	-0.71844700000000
C	1.92615600000000	3.13567500000000	-1.41654100000000
H	2.59755000000000	-3.79786500000000	2.13135100000000
H	3.69874700000000	-5.23036400000000	-1.82070000000000

H	2.15342000000000	-3.55619800000000	-2.87672400000000
Cl	-1.61225200000000	-2.37063000000000	3.21153700000000
Cl	-4.28999200000000	-3.34485200000000	1.82613500000000
Cl	-4.56364400000000	-3.20209300000000	-1.33662100000000
Cl	-2.15738100000000	-2.08141100000000	-3.06721300000000
H	-1.81240200000000	1.25324200000000	2.76385400000000
H	-3.99145100000000	1.96748500000000	1.72170800000000
H	-4.20612900000000	2.09040800000000	-0.79517800000000
H	-2.23930300000000	1.49884900000000	-2.25421300000000
H	2.26366100000000	2.93890500000000	2.49606100000000
H	3.42694600000000	4.75664600000000	1.21610300000000
H	3.21211700000000	4.88264200000000	-1.27192800000000
H	2.15617400000000	-0.24183100000000	-1.33493300000000
H	0.30334200000000	1.08766100000000	-2.38043300000000
H	0.71274400000000	0.84693200000000	2.41898000000000
H	0.43373700000000	-1.63148000000000	-2.51873500000000
H	0.85457500000000	-1.86690100000000	2.26748400000000
C	1.28482400000000	-0.39065100000000	0.67109300000000
H	2.35397000000000	-0.34900500000000	0.94609900000000
H	1.83374100000000	3.19052600000000	-2.51054400000000
H	3.91887300000000	-5.34956700000000	0.66668700000000
Ag	-3.71439800000000	-0.50045800000000	0.31319100000000

4·Ag⁺ E=-6907.359093339177 Hartree

C	0.36998100000000	-1.46815200000000	0.98029500000000
C	-0.01982500000000	-2.46932400000000	-0.15966100000000
C	-0.66327400000000	-3.48732900000000	2.16384300000000
C	-0.83173700000000	-1.03536800000000	3.19623300000000
C	-0.20573000000000	-0.01749900000000	0.87081400000000
C	0.37306600000000	-4.31929300000000	1.40874000000000
C	0.96454300000000	-5.50750300000000	1.85409600000000
C	1.91957200000000	-6.14113200000000	1.03448100000000
C	2.26629500000000	-5.59282800000000	-0.21408600000000
C	1.66375600000000	-4.40204400000000	-0.66605200000000
C	0.72165700000000	-3.76812600000000	0.15301800000000
C	-1.82649000000000	-3.39505200000000	1.20752300000000
C	-3.13605700000000	-3.84361200000000	1.45511200000000
C	-4.11577400000000	-3.81290500000000	0.39924100000000
C	-3.75900100000000	-3.25885800000000	-0.88121300000000
C	-2.43097000000000	-2.74054900000000	-1.08187800000000
C	-1.47679200000000	-2.84479200000000	-0.05421600000000
C	-2.03685100000000	-0.54885200000000	2.41727700000000
C	-3.35316200000000	-0.48636400000000	2.89013400000000

C	-4.34772100000000	0.18382700000000	2.12074600000000
C	-4.00526400000000	0.74110900000000	0.84483300000000
C	-2.67176700000000	0.61894600000000	0.35488300000000
C	-1.69549500000000	0.00422900000000	1.14819200000000
C	0.42126000000000	0.73619700000000	2.04377700000000
C	0.08313300000000	0.18483700000000	3.30217300000000
C	0.58643300000000	0.74634300000000	4.48123400000000
C	1.43544300000000	1.86841700000000	4.39776000000000
C	1.77169900000000	2.41582100000000	3.14739400000000
C	1.26440600000000	1.85026700000000	1.96029600000000
H	0.69050700000000	-5.93611300000000	2.82710900000000
H	3.00806200000000	-6.09879400000000	-0.84538300000000
H	1.92962100000000	-3.97834100000000	-1.64324900000000
C	-3.50937800000000	-4.27749700000000	2.76425300000000
C	-5.42130500000000	-4.36897700000000	0.60549200000000
C	-4.71057300000000	-3.25131100000000	-1.95306900000000
C	-2.09981000000000	-2.07395400000000	-2.30163600000000
H	-3.61306800000000	-0.89515100000000	3.87513800000000
H	-5.33565800000000	0.38424300000000	2.55894100000000
H	-4.72929300000000	1.37066400000000	0.30852100000000
H	-2.40685400000000	1.06327200000000	-0.61332800000000
H	0.32248900000000	0.32069600000000	5.45886500000000
H	1.83192900000000	2.31897600000000	5.31625400000000
H	2.42881200000000	3.29333400000000	3.09332900000000
H	1.46715800000000	-1.36629600000000	0.91376100000000
H	0.04519800000000	0.43627200000000	-0.10436400000000
H	-1.10856800000000	-1.44165300000000	4.18425100000000
H	0.23607200000000	-2.06380300000000	-1.15345000000000
H	-0.94958400000000	-3.94133400000000	3.12738400000000
C	-0.00956500000000	-2.07877000000000	2.36917400000000
H	0.91141100000000	-2.26911000000000	2.94866400000000
H	1.52608900000000	2.27944200000000	0.98392800000000
H	2.39075400000000	-7.07274700000000	1.37154800000000
N	-3.79164900000000	-4.57668400000000	3.86340100000000
N	-6.49678300000000	-4.80302900000000	0.78669100000000
N	-5.49577300000000	-3.22091200000000	-2.82503300000000
N	-1.80645400000000	-1.47565000000000	-3.26774300000000
Ag	-4.71242600000000	-1.45995000000000	0.47783400000000

5·Ag⁺ E=-6759.730923687140 Hartree

C	1.12928465453013	-0.29777049142563	-0.88747749068068
C	0.50593908897199	-1.63310622908383	-1.42240906147950
C	0.70872325782646	-1.74472267344592	1.17916810391391

C	0.63935368499426	0.92716685042288	1.30088351198095
C	0.42690795702346	1.04312417146192	-1.28247999976864
C	1.56958510068037	-2.78680889449153	0.46694520165106
C	2.42041561825805	-3.71983048851993	1.07135848682684
C	3.16461170526708	-4.60020211035077	0.25988013597183
C	3.05545703613401	-4.54061070174962	-1.14029768554974
C	2.20075486801587	-3.59887337108467	-1.74902706009238
C	1.46064692017138	-2.72569156588381	-0.94307041510387
C	-0.69983656443017	-1.98649666698694	0.68229711663831
C	-1.80492827333088	-2.33841526312444	1.46502146767209
C	-3.04451244439403	-2.66221260412892	0.83623196591530
C	-3.15005615003771	-2.60992527001761	-0.58803024804394
C	-2.02205139911626	-2.23082779223615	-1.36823762521030
C	-0.80987215216622	-1.92988033666527	-0.73715505197491
C	-0.79042338033121	1.16394215374187	0.84006114306531
C	-1.87101936004797	1.49511578463923	1.67669504306013
C	-3.11236486299587	1.90958073339919	1.06721289052203
C	-3.29059965909548	1.78738560080162	-0.35952444445071
C	-2.13552304919714	1.51058257124045	-1.19249807175849
C	-0.91104696780526	1.20369953660441	-0.57521431509787
C	1.32979307747217	2.13555769998459	-0.71227573267438
C	1.44877042682524	2.07147505971171	0.69689039719185
C	2.25765395596217	2.98556367037469	1.38149991698023
C	2.94581193460390	3.97857303304600	0.65379739204363
C	2.82739119637002	4.04325073261788	-0.74493359678899
C	2.02025838905736	3.11499468400567	-1.43529010940830
H	2.50726315296668	-3.76585250570941	2.16627609948138
H	3.63658526735597	-5.23186121684597	-1.76461043000158
H	2.11573895309170	-3.55177047576669	-2.84412977935137
H	-1.71552969294446	-2.40837476533380	2.55733345464012
H	-3.87391909686392	-3.06692737800247	1.43242125033235
H	-4.06867988895598	-2.95459735483110	-1.08152525657499
H	-2.10412503801243	-2.20293422655728	-2.46307332143566
N	-1.79662533884088	1.63813922770962	3.07877061016548
N	-4.11121121981202	2.48830024076950	1.84649900697258
N	-4.45366014823933	2.30563030717535	-0.96336849518003
N	-2.34423077050867	1.54765147222030	-2.57952221258533
H	2.35711820540339	2.93123214463787	2.47529840986566
H	3.57684825831824	4.70372873642929	1.18447425474745
H	3.36591712816703	4.81915906218560	-1.30471916403743
H	2.14178678919605	-0.25067092618602	-1.32686139230685
H	0.35209161028642	1.12429957955183	-2.38263182360926
H	0.73713608686280	0.88704499141095	2.40139512728561
H	0.40923254825437	-1.61392466764959	-2.52292284575124
H	0.78253042065399	-1.81952340096637	2.27963221973472

C	1.25261008888015	-0.36673105989874	0.67128894082295
H	2.32264170286834	-0.35358656994196	0.94755258983971
H	1.93585970332275	3.16185707011078	-2.53087260108420
H	3.83076200563220	-5.33789505493375	0.72651119315771
H	-4.58212719975134	3.27983796900956	1.39560824691475
H	-3.75568392900263	2.73906421705964	2.77662965734832
H	-4.60979676043377	1.93726125904570	-1.90663526704501
H	-5.30261927836916	2.22194182122976	-0.39895009003950
H	-1.53209104586526	1.27669181090035	-3.13525821152354
H	-2.72815135151974	2.43692854022331	-2.91880851441219
H	-0.85114466801333	1.66437094306361	3.46169190898523
H	-2.39364534281051	1.00647556373229	3.62079669475181
Ag	-3.53030676053239	-0.43329417669924	0.32735587454156

6·Ag⁺ E=-6935.658494946133 Hartree

C	1.10475297372819	-0.30410675524873	-0.88232713914665
C	0.48518426584266	-1.64286366756424	-1.41372393008292
C	0.73556115697632	-1.76734107922681	1.18687580113339
C	0.59252552645746	0.90374556737044	1.31464883799176
C	0.39697153842244	1.03338691128142	-1.28850216019505
C	1.59726582843851	-2.78471462891542	0.44995359539453
C	2.46417112822907	-3.70571927232117	1.03470269894822
C	3.20471655557871	-4.57783325109195	0.20740639285703
C	3.06616597141379	-4.51455651123860	-1.19173117692488
C	2.18631191078641	-3.57803960100072	-1.77715927350559
C	1.45891840636722	-2.72084577685357	-0.95374066399871
C	-0.67738445178285	-2.03902798655380	0.71230276496495
C	-1.75786144715823	-2.42501129147285	1.51266797186741
C	-2.99790519254920	-2.77081520349841	0.90577394011397
C	-3.13897894466924	-2.69560610806550	-0.51520833502216
C	-2.03459178948708	-2.27594039323086	-1.31402987411541
C	-0.81480386209477	-1.96501614631155	-0.70349000311429
C	-0.82972119483951	1.10065667690454	0.83264818252976
C	-1.95491752762606	1.30965006809427	1.63817912685512
C	-3.20873111802181	1.62637343410347	1.03691255835171
C	-3.31167932350818	1.70414355713799	-0.38734934484525
C	-2.16355539788885	1.46196502420857	-1.19287717131501
C	-0.93545922258665	1.17673375771375	-0.58585266910013
C	1.27642720450828	2.13507811276259	-0.69734744942433
C	1.37939253772772	2.06729488577017	0.71253267025794
C	2.16346306761917	2.99284765088382	1.41147365726181
C	2.84614532009843	3.99595523696766	0.69372804640262
C	2.74293332359083	4.06429316463719	-0.70660529775455

C	1.95609825914183	3.12986993609668	-1.41045165711463
F	2.61086897295821	-3.77787175805022	2.35837376945831
F	3.76426952579819	-5.34112414947943	-1.95819122790902
F	2.07014995159105	-3.53143243040929	-3.10484972276102
H	-1.64662518776237	-2.50088455256122	2.60234577780955
H	-3.80658322512786	-3.19844886410908	1.51431462979764
H	-4.04879886953413	-3.07987487687631	-0.99742429379977
H	-2.13841307273862	-2.24003676793001	-2.40701096596803
H	-1.87252341148758	1.27382099402663	2.73290546366048
H	-4.05604422208740	1.93299188483820	1.66577136826675
H	-4.24341074949448	2.05685065799233	-0.85064676255935
H	-2.24135620264805	1.53944862444027	-2.28558180677272
H	2.24602166797067	2.93905696895178	2.50624590402634
H	3.45905924846549	4.72930789951939	1.23398253970164
H	3.27527406031668	4.85098754449480	-1.25687858937826
H	2.11328390602440	-0.24945435399471	-1.32902699294513
H	0.30264315424916	1.11507062096307	-2.38608948587041
H	0.66114476757910	0.87456131740242	2.41705698989774
H	0.37329155085214	-1.62643714199204	-2.51107047032629
H	0.83619896787857	-1.85364900492424	2.28248287077253
C	1.23816501244068	-0.37383765653016	0.67717854943687
H	2.30767906526560	-0.32843342686554	0.95047641276074
H	1.87765480136417	3.18265262323507	-2.50568842268035
F	4.03193810673491	-5.46353344314516	0.74542118922540
Ag	-3.66523232132316	-0.55685102033494	0.30110217688570

7·Ag⁺ E=-8385.664734103779 Hartree

C	1.09254100000000	-0.29519300000000	-0.88055200000000
C	0.46736600000000	-1.63199800000000	-1.40858500000000
C	0.71509200000000	-1.75626500000000	1.18510700000000
C	0.58604400000000	0.91357200000000	1.31640200000000
C	0.38683700000000	1.04313500000000	-1.28698300000000
C	1.58009500000000	-2.77711400000000	0.45185800000000
C	2.45797100000000	-3.69719800000000	1.03782700000000
C	3.21054600000000	-4.57282200000000	0.21335500000000
C	3.07308300000000	-4.50792100000000	-1.19620400000000
C	2.18483400000000	-3.56674000000000	-1.77736900000000
C	1.44404600000000	-2.71220100000000	-0.95154100000000
C	-0.69710100000000	-2.02754800000000	0.71217100000000
C	-1.77670900000000	-2.41552500000000	1.51301300000000
C	-3.01618700000000	-2.76026400000000	0.90435500000000
C	-3.15608800000000	-2.68493000000000	-0.51699400000000
C	-2.05138600000000	-2.26659700000000	-1.31574800000000

C	-0.83325200000000	-1.95402000000000	-0.70243400000000
C	-0.83658100000000	1.11291700000000	0.83632300000000
C	-1.96055400000000	1.32170100000000	1.64351800000000
C	-3.21514300000000	1.63841200000000	1.04411400000000
C	-3.32026200000000	1.71617800000000	-0.38001500000000
C	-2.17328900000000	1.47371100000000	-1.18733500000000
C	-0.94433300000000	1.18860100000000	-0.58206900000000
C	1.26992000000000	2.14261700000000	-0.69721300000000
C	1.37518500000000	2.07463200000000	0.71251500000000
C	2.16368400000000	2.99757900000000	1.40991600000000
C	2.84826600000000	3.99838200000000	0.69076700000000
C	2.74269900000000	4.06694600000000	-0.70937800000000
C	1.95162600000000	3.13498400000000	-1.41172800000000
Cl	2.62893100000000	-3.76384200000000	2.76870000000000
Cl	3.98401100000000	-5.57467600000000	-2.20221300000000
Cl	2.02134800000000	-3.47367300000000	-3.50735500000000
H	-1.66462900000000	-2.49394200000000	2.60233500000000
H	-3.82573100000000	-3.18793600000000	1.51170900000000
H	-4.06632500000000	-3.06808200000000	-0.99924500000000
H	-2.15265000000000	-2.23315000000000	-2.40894200000000
H	-1.87654900000000	1.28536900000000	2.73809600000000
H	-4.06162500000000	1.94476500000000	1.67421400000000
H	-4.25236300000000	2.06982300000000	-0.84190400000000
H	-2.25274200000000	1.55066400000000	-2.27995300000000
H	2.24840000000000	2.94331700000000	2.50447900000000
H	3.46479100000000	4.72960500000000	1.22979100000000
H	3.27679100000000	4.85169100000000	-1.26072900000000
H	2.09964400000000	-0.24423100000000	-1.33101200000000
H	0.29123200000000	1.12420000000000	-2.38441200000000
H	0.65649200000000	0.88386800000000	2.41858500000000
H	0.36063800000000	-1.62010800000000	-2.50589700000000
H	0.81923100000000	-1.84654200000000	2.27893800000000
C	1.22638400000000	-0.36562700000000	0.67747700000000
H	2.29557500000000	-0.32678800000000	0.95331300000000
H	1.87171100000000	3.18751000000000	-2.50685300000000
Cl	4.28950900000000	-5.71606900000000	0.92573500000000
Ag	-3.67667000000000	-0.54352600000000	0.30356000000000

8·Ag⁺ E=-6907.372112260877 Hartree

C	1.10943200000000	-0.31339200000000	-0.88467300000000
C	0.47925800000000	-1.65158000000000	-1.41430000000000
C	0.73713600000000	-1.77748400000000	1.18492000000000
C	0.59576800000000	0.89077800000000	1.31259100000000

C	0.39986500000000	1.02150200000000	-1.29222200000000
C	1.59951300000000	-2.78974800000000	0.44368000000000
C	2.48150400000000	-3.71504900000000	1.03345900000000
C	3.23557600000000	-4.59709400000000	0.20012600000000
C	3.09312300000000	-4.53123300000000	-1.21209000000000
C	2.19646000000000	-3.58322900000000	-1.79345300000000
C	1.45817900000000	-2.72469400000000	-0.95697500000000
C	-0.67710500000000	-2.05157500000000	0.71343200000000
C	-1.75311000000000	-2.43650000000000	1.52021600000000
C	-2.99595500000000	-2.77295500000000	0.91539800000000
C	-3.14154600000000	-2.69641600000000	-0.50484400000000
C	-2.03904100000000	-2.28476100000000	-1.30963800000000
C	-0.81846200000000	-1.97635300000000	-0.69935800000000
C	-0.82718400000000	1.08662700000000	0.82946600000000
C	-1.95107900000000	1.30143500000000	1.63580700000000
C	-3.20241400000000	1.62879200000000	1.03432700000000
C	-3.30503900000000	1.70756100000000	-0.38996500000000
C	-2.15946200000000	1.45578000000000	-1.19613200000000
C	-0.93292800000000	1.16380800000000	-0.58861300000000
C	1.28054500000000	2.12239400000000	-0.70003100000000
C	1.38330700000000	2.05439500000000	0.70983100000000
C	2.16785000000000	2.97880200000000	1.40972800000000
C	2.85033700000000	3.98169200000000	0.69137700000000
C	2.74729300000000	4.05023700000000	-0.70903700000000
C	1.96066700000000	3.11632500000000	-1.41387200000000
C	2.60095500000000	-3.75767200000000	2.45976200000000
C	3.84081800000000	-5.41216400000000	-2.05444900000000
C	2.03006200000000	-3.49220000000000	-3.21261600000000
H	-1.63654800000000	-2.51747200000000	2.60883400000000
H	-3.80550600000000	-3.19549100000000	1.52639200000000
H	-4.05501500000000	-3.07642600000000	-0.98375800000000
H	-2.14443300000000	-2.25260100000000	-2.40246700000000
H	-1.86878000000000	1.26700200000000	2.73059700000000
H	-4.04655400000000	1.94351100000000	1.66357700000000
H	-4.23407700000000	2.06752700000000	-0.85316200000000
H	-2.23689000000000	1.53556500000000	-2.28869000000000
H	2.25111300000000	2.92494200000000	2.50431900000000
H	3.46357100000000	4.71468100000000	1.23154800000000
H	3.28009700000000	4.83669200000000	-1.25899900000000
H	2.11585300000000	-0.25930000000000	-1.33666300000000
H	0.30718800000000	1.10208600000000	-2.38976800000000
H	0.66581400000000	0.86027600000000	2.41460900000000
H	0.36492700000000	-1.63361100000000	-2.51172800000000
H	0.84298500000000	-1.86401000000000	2.28005800000000
C	1.24476800000000	-0.38303200000000	0.67311400000000

H	2.31365700000000	-0.33587300000000	0.94919800000000
H	1.88309100000000	3.16929400000000	-2.50904400000000
C	4.12751800000000	-5.54481300000000	0.79207200000000
N	4.85525900000000	-6.31814500000000	1.29064500000000
N	2.64484700000000	-3.73736100000000	3.63230700000000
N	4.44763700000000	-6.12988400000000	-2.75651100000000
N	1.84080800000000	-3.36200100000000	-4.36340300000000
Ag	-3.67370700000000	-0.55367200000000	0.30597700000000

9·Ag⁺ E=-6759.722250986202 Hartree

C	1.11791800000000	-0.37734600000000	-0.85738700000000
C	0.53020300000000	-1.72428000000000	-1.40392400000000
C	0.67939500000000	-1.83176600000000	1.20210400000000
C	0.62315600000000	0.84890200000000	1.32456500000000
C	0.39236200000000	0.94585600000000	-1.26985400000000
C	1.56302500000000	-2.86725700000000	0.50925600000000
C	2.40879900000000	-3.79240000000000	1.13295200000000
C	3.18171200000000	-4.66346600000000	0.33841000000000
C	3.10585900000000	-4.60223000000000	-1.06395400000000
C	2.25530700000000	-3.66930900000000	-1.69174900000000
C	1.48619000000000	-2.80515900000000	-0.90293000000000
C	-0.71657900000000	-2.08646500000000	0.67531800000000
C	-1.83644200000000	-2.44583800000000	1.43380300000000
C	-3.05926600000000	-2.77987600000000	0.77973800000000
C	-3.13737200000000	-2.72203900000000	-0.64734400000000
C	-1.99551000000000	-2.33441300000000	-1.40190100000000
C	-0.79664900000000	-2.03380200000000	-0.74649800000000
C	-0.80381300000000	1.06208600000000	0.86576800000000
C	-1.91424000000000	1.30201300000000	1.68419900000000
C	-3.17212600000000	1.61811600000000	1.09760400000000
C	-3.30138500000000	1.66091100000000	-0.32661600000000
C	-2.16508500000000	1.38844900000000	-1.14650100000000
C	-0.92974700000000	1.10305700000000	-0.55437900000000
C	1.26874900000000	2.06010100000000	-0.70491000000000
C	1.40405900000000	2.00799800000000	0.70019200000000
C	2.23642500000000	2.93646100000000	1.36636100000000
C	2.87632900000000	3.94504700000000	0.59259300000000
C	2.70917400000000	3.99729300000000	-0.81842700000000
C	1.90337200000000	3.02816100000000	-1.49309200000000
H	2.46873200000000	-3.84005500000000	2.22973100000000
H	3.70932100000000	-5.28599100000000	-1.67524300000000
H	2.19614900000000	-3.62108000000000	-2.78849500000000
H	-1.77171400000000	-2.51159600000000	2.52806700000000

H	-3.89314800000000	-3.20227300000000	1.35783800000000
H	-4.04059800000000	-3.07949600000000	-1.16057300000000
H	-2.05257500000000	-2.30667500000000	-2.49846200000000
N	2.41717000000000	2.93779600000000	2.75079300000000
N	3.65225500000000	4.97788800000000	1.19194800000000
N	3.35274000000000	4.99984500000000	-1.51712700000000
H	2.13053300000000	-0.30039700000000	-1.29145500000000
H	0.30760800000000	1.03762400000000	-2.36618600000000
H	0.68298100000000	0.81409100000000	2.42830800000000
H	0.45650300000000	-1.70387500000000	-2.50574000000000
H	0.72968800000000	-1.90579900000000	2.30404500000000
C	1.23151700000000	-0.44993900000000	0.70181300000000
H	2.29951600000000	-0.43820500000000	0.98584200000000
N	1.72419200000000	3.04187600000000	-2.91357200000000
H	3.84358600000000	-5.39545500000000	0.81991700000000
H	2.59966100000000	3.18285200000000	-3.42754800000000
H	1.02651800000000	3.71788600000000	-3.24390500000000
H	2.94522700000000	5.25524300000000	-2.41653700000000
H	3.64105600000000	5.78247100000000	-0.92045000000000
H	4.66900100000000	4.84482300000000	1.18102900000000
H	3.32498100000000	5.28657800000000	2.10994700000000
H	3.32202600000000	3.30245700000000	3.05489700000000
H	-1.81527300000000	1.28499100000000	2.77804900000000
H	-2.25864100000000	1.43944600000000	-2.23968400000000
H	-4.23369000000000	2.02355000000000	-0.78143700000000
H	-4.01253900000000	1.93015200000000	1.73239200000000
H	2.16247100000000	2.08277200000000	3.24235200000000
Ag	-3.65323000000000	-0.57332300000000	0.28369000000000

10·Ag⁺ E=-7333.336122839294 Hartree

C	1.11162874944163	-0.29668136767622	-0.88348117575197
C	0.49044986352562	-1.63231078021246	-1.41658840491852
C	0.73800843630479	-1.75741966807530	1.18549163169277
C	0.60509050083116	0.90972454926008	1.31642918899533
C	0.40431779959026	1.04060226676510	-1.28741079985948
C	1.59376738565587	-2.78025029961533	0.44905489909117
C	2.45529201903405	-3.70502285154976	1.03543766280676
C	3.19276315343465	-4.58047483970923	0.20825348242027
C	3.05669443431338	-4.51601138096923	-1.19110908261453
C	2.18217137054989	-3.57498440820626	-1.77824888744817
C	1.45781925860547	-2.71528631318639	-0.95507556690497
C	-0.67486935695314	-2.02019796786529	0.70527377432157
C	-1.73953734027976	-2.42980167026200	1.50576543429751

C	-2.9766693924113	-2.79634399599077	0.90091786013746
C	-3.12314550411925	-2.70916095927109	-0.52309290953241
C	-2.01429604594437	-2.28344703143442	-1.32022068141641
C	-0.81036109950260	-1.94727078618427	-0.70415102546521
C	-0.81762696431024	1.10754675818541	0.83776609379492
C	-1.94014262376630	1.32230198677197	1.64729570028980
C	-3.19208728086148	1.65142820794415	1.04908591387539
C	-3.29975697310330	1.72651451889696	-0.37645633493051
C	-2.15480892852826	1.47345077087075	-1.18658920530789
C	-0.92613840676901	1.18302170808461	-0.58136402765559
C	1.28405122324568	2.14265372488009	-0.69670520180956
C	1.39000516639117	2.07398845871454	0.71273342213181
C	2.17363335397527	3.00017044631974	1.41132072942497
C	2.85335221602813	4.00466576423263	0.69280527460193
C	2.74726634985584	4.07391835045081	-0.70731146719155
C	1.96049021450725	3.13906449231325	-1.41063521228524
F	2.59994452444533	-3.77761570656271	2.35849844948767
F	3.75180066274922	-5.34500119550352	-1.95652350504353
F	2.06856301396102	-3.52686658102138	-3.10532365330617
F	-1.62904891699385	-2.52367843416526	2.82585860313710
F	-3.93994649428829	-3.35313113352386	1.62241039424606
F	-4.20942070176889	-3.21540950297728	-1.09883200054700
F	-2.16085121608593	-2.25230143475631	-2.63948886164428
H	-1.85532783937449	1.28537165571537	2.74182938313795
H	-4.03875643964598	1.95670158931655	1.67918554375902
H	-4.22973691418554	2.08825688934929	-0.83655706092644
H	-2.23547982168283	1.55077828493082	-2.27914712507092
H	2.25820984545282	2.94578511799319	2.50586028416806
H	3.46611245791294	4.73856291758402	1.23242988183009
H	3.27722861455589	4.86193410986724	-1.25791120557169
H	2.11974990280192	-0.24398856569066	-1.33103536741136
H	0.30707411049244	1.12325470514702	-2.38455038385094
H	0.67618122604483	0.87972047258489	2.41849945352143
H	0.37302485697264	-1.61733662998945	-2.51198103340019
H	0.82896133941099	-1.84721107438718	2.28022696376904
C	1.24613386748393	-0.36782039926561	0.67661917554353
H	2.31592325305918	-0.32808140333387	0.94926476339907
H	1.87972004085178	3.19289463284185	-2.50559991242779
F	4.01463579512782	-5.46966823709042	0.74705496481679
Ag	-3.63087919920822	-0.51558476054480	0.25703516359483

\compound{11}{ } E=\$-10233.357804992873 Hartree

\begin{verbatim}

C	1.13303943234859	-0.30206106881440	-0.88482045260690
C	0.52754715950284	-1.64203839607049	-1.41899504026256

C	0.75507998556075	-1.76847599290057	1.17061467100198
C	0.62102281302362	0.89007896340027	1.32001120335081
C	0.39584677841885	1.01975672050430	-1.28288827646309
C	1.61730486052366	-2.79473790418944	0.44526651978977
C	2.48315173317728	-3.72113992384258	1.03919491761144
C	3.23762257881905	-4.59876612663604	0.21829637283586
C	3.11349266678869	-4.52978036813012	-1.19293395884192
C	2.23620267935865	-3.58260662548124	-1.78121617734074
C	1.49483883454256	-2.72591398929797	-0.95809566451895
C	-0.65777666544728	-2.02262431312898	0.68639833681422
C	-1.75576779834891	-2.36065982703513	1.48621123689273
C	-3.00407314793440	-2.69464796347825	0.87043235283351
C	-3.12885727787350	-2.62757769851396	-0.56236847210700
C	-2.00306709131412	-2.22601745945250	-1.34995761261151
C	-0.78107622371194	-1.95499405963068	-0.72357231484032
C	-0.80837529398885	1.07688360517420	0.85483071352186
C	-1.91862724313092	1.30694691239775	1.67598267100490
C	-3.17078196911465	1.65758457572098	1.09102602961961
C	-3.29406294271094	1.72778300687846	-0.33465808475417
C	-2.16351376091243	1.44634161935744	-1.15650050544750
C	-0.93113064275877	1.14712703167273	-0.56374740513973
C	1.26343249238309	2.13539512059011	-0.69853273051143
C	1.38558215575296	2.06505499372794	0.70980576567137
C	2.16324097198552	3.00102510587997	1.40180534516347
C	2.82021298513725	4.01710364013774	0.67832962973083
C	2.69758884974062	4.08815330002606	-0.72030901770052
C	1.91715460215589	3.14319583632288	-1.41730001954479
Cl	2.63674063253725	-3.79089739972821	2.77031677185027
Cl	4.02731635796708	-5.59912348885776	-2.19257462855006
Cl	2.08725596447365	-3.48289788679793	-3.51079575318887
Cl	-1.62753009802542	-2.36174270173652	3.21338357935870
Cl	-4.31447763831605	-3.31703625194496	1.82900316913992
Cl	-4.58909301677011	-3.17211854217445	-1.33304756559178
Cl	-2.17473340601370	-2.06866724231579	-3.06607130225092
H	-1.82154906330940	1.27171434008354	2.76912599840406
H	-3.99995376706417	1.99180076445179	1.72995521895368
H	-4.21771004033567	2.11552657801357	-0.78671472730697
H	-2.25494285697861	1.51780011702114	-2.24859465617366
H	2.26068703501655	2.94524852330382	2.49514944094527
H	3.42826862759691	4.75856644954658	1.21296148987209
H	3.20991974915636	4.88514121231524	-1.27468123214321
H	2.13766697932696	-0.23179516961713	-1.33813246508126
H	0.28680832464983	1.09957524567744	-2.37881635370906
H	0.70249563706393	0.85815040958613	2.42094568437943
H	0.41994332196516	-1.62965624220053	-2.51427225509064

H	0.84085972785221	-1.86421672277769	2.26369311964764
C	1.26912960019888	-0.37831883741545	0.67203789492349
H	2.33782315901600	-0.34130826480202	0.94959620664130
H	1.82375000072842	3.19790386926105	-2.51117719740181
Cl	4.30334738055808	-5.74950963992510	0.93715639082392
Ag	-3.73417813326728	-0.47705583415525	0.31924913839723

12·Ag⁺ E=-7276.755116584327 Hartree

C	0.35575138904256	-1.48541625655894	0.96602613903896
C	-0.03992089550269	-2.49050541665005	-0.17513393101076
C	-0.67930713696680	-3.50734049123800	2.14993802953870
C	-0.84414174963633	-1.05602549857093	3.18377233220289
C	-0.22247546220230	-0.03748993962698	0.85458720059380
C	0.37147170420774	-4.31867609551241	1.40258055788287
C	0.99878709436569	-5.48781098216209	1.87587857108979
C	1.99261966885921	-6.12051120960887	1.06904600963574
C	2.33939143107737	-5.56818209136256	-0.19480527364021
C	1.69418328808510	-4.38074887830709	-0.65647154117004
C	0.71568805719827	-3.77152193076931	0.15305713064216
C	-1.84585213642014	-3.41159188480439	1.19425716724271
C	-3.15900506000858	-3.84216499095419	1.45661056144377
C	-4.14401740940852	-3.78927445106924	0.40919338264418
C	-3.79035515719660	-3.23339833913729	-0.87186961663635
C	-2.45821141288442	-2.73592444743190	-1.08548329995063
C	-1.49974421915563	-2.86328400577936	-0.06394347023460
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H	2.43162912967227	3.26097367154337	3.07127911459476
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13·Ag⁺ E=-6981.489031625473 Hartree

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