Supporting Information for the manuscript:

Infrared Multiple Photon Dissociation of Cesium Iodide Clusters Doped with Mono-, Di- and Triglycine

Jakob Heller, Milan Ončák, Nina K. Bersenkowitsch, Christian van der Linde, and Martin K. Beyer

Institut für Ionenphysik und Angewandte Physik, Leopold-Franzens-Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria

E-mail: martin.beyer@uibk.ac.at

Lookup table for the evaluation of multiphoton cross sections

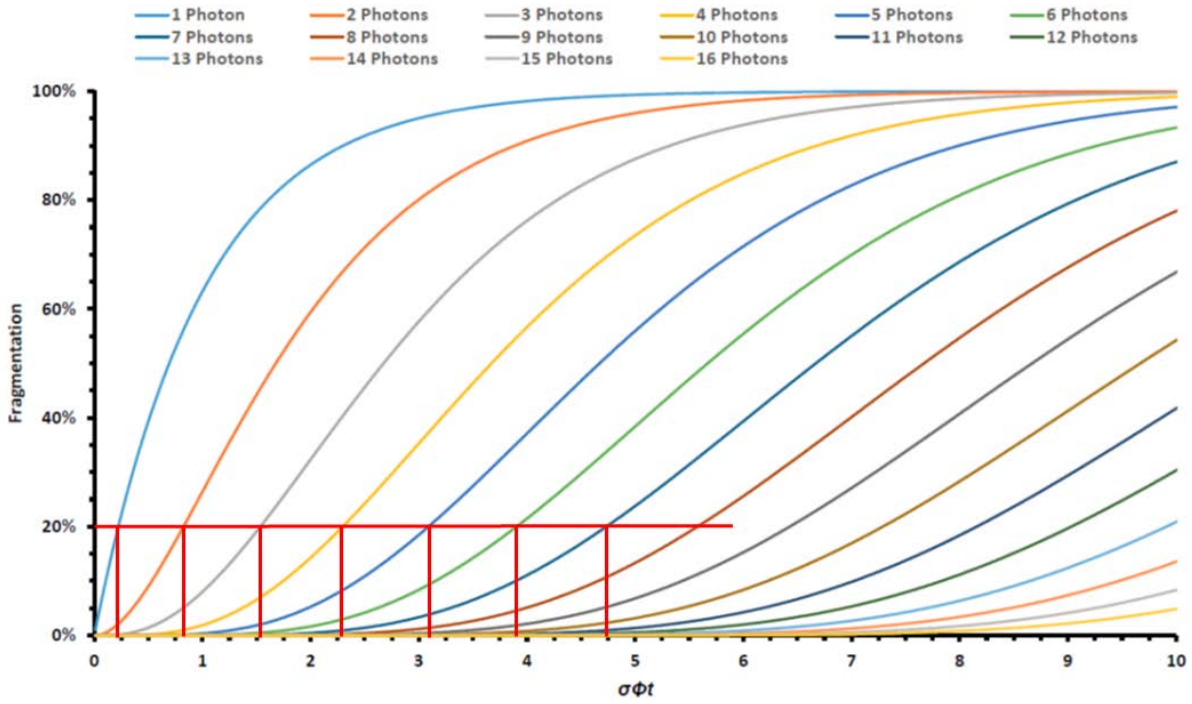

Figure S1: Graphical representation of the lookup table used for the quantitative analysis of multiphoton absorption.

Quantitative data analysis is based on the consecutive first-order reactions shown in Figure S1. Assuming that the absorption cross section does not change during the absorption of multiple photons, Figure S1 shows the kinetics of IR photon absorption. If fragmentation occurs upon absorption of the k^{th} photon, the value of $\sigma\Phi t$ is obtained readily from the graph, as shown for 20% fragmentation yield for 1 to 7 photons. Photon flux Φ is measured with a power meter, t is set in the control software, thus σ can be calculated from $\sigma\Phi t$. This graphical scheme is implemented in our data analysis software with a densely spaced lookup table.

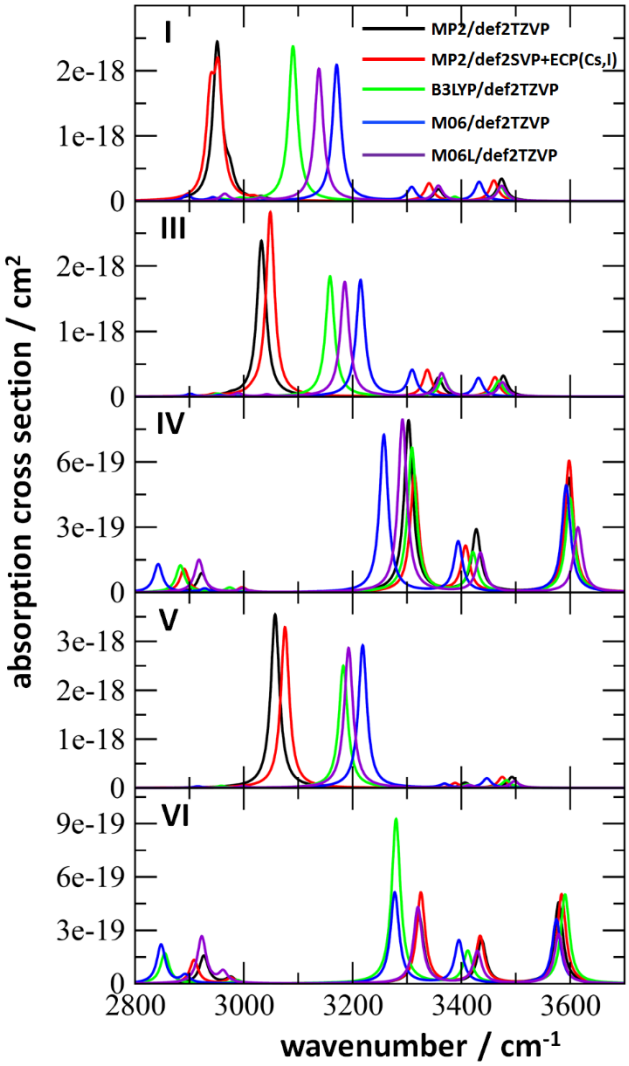

Figure S2: Vibrational spectra of five $Cs_3I_2.G^+$ isomers calculated at various levels of theory (see Figure 1 for structures). The "def2SVP+ECP(Cs,I)" basis set stands for ECP54SDF on Cs, ECP46MDF on I, and def2SVP on all other atoms. The following factors were used to scale the calculated peak positions: 0.963 (MP2/def2TZVP), 0.942 (MP2/def2SVP+ECP(Cs,I)), 0.966 (B3LYP/def2TZVP), 0.951 (M06/def2TZVP), 0.966 (M06L/def2TZVP).

Table S1: Relative energy of four $Cs_3I_2.G^+$ isomers at various levels of theory, the def2TZVP basis set was used unless stated otherwise. The "def2SVP+ECP(Cs,I)" basis set stands for ECP54SDF on Cs, ECP46MDF on I, and def2SVP on all other atoms. See Figure 1 for the respective structures.

isomer	MP2	MP2/def2SVP+ECP(Cs,I)	B3LYP	M06	M06L
I	0.0	0.0	0.0	0.0	0.0
III	45.7	24.1	27.1	48.2	47.4
IV	26.5	25.9	13.6	21.7	23.5
V	58.6	27.4	19.2	55.0	56.4
VI	41.1	38.2	28.6	37.2	38.1

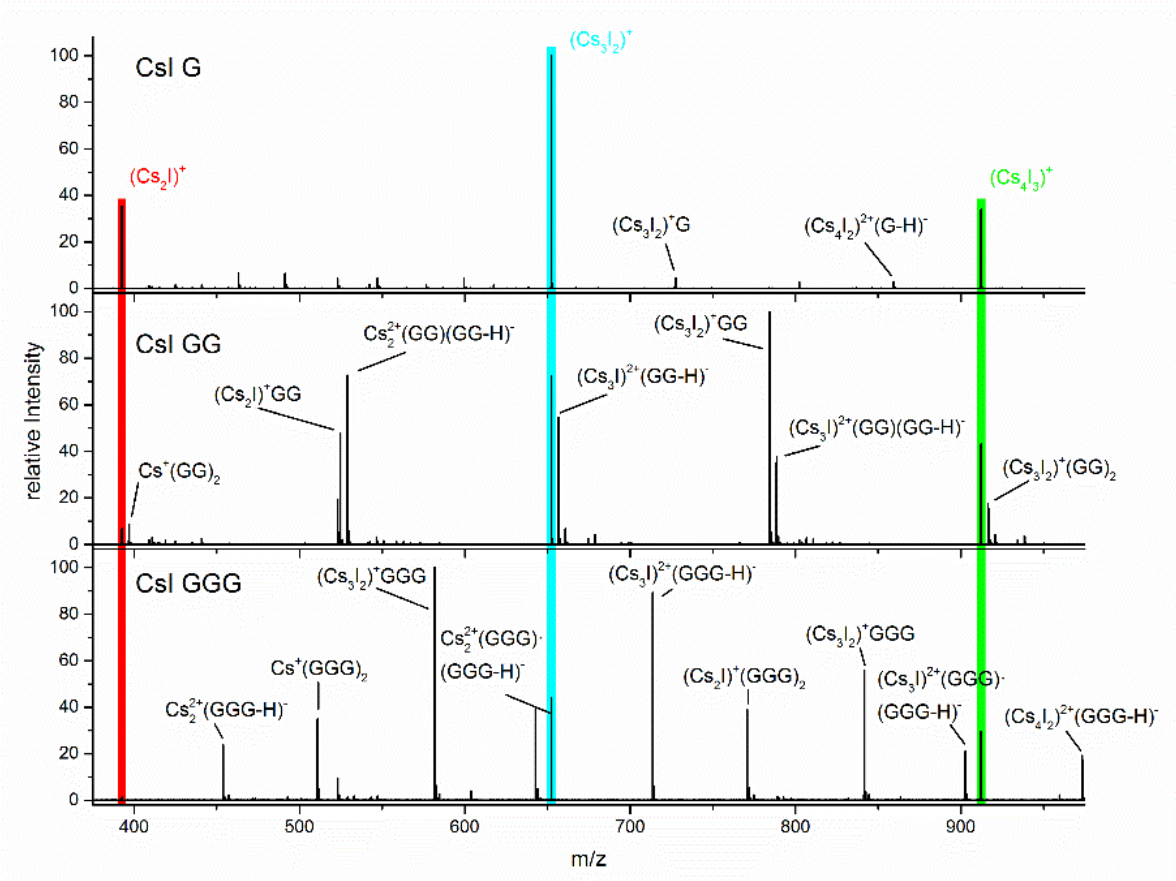

Figure S3: Mass spectra of CsI mixed with glycine (G) (top), digylcine GG (middle) and triglycine GGG (bottom). Complexes consisting of neutral and deprotonated peptides are found.

Table S2: Identified complexes in ESI of CsI with G.

Ion	m_{meas} (Da)	m_{exact} (Da)	Δm (ppm)	Δm (Da)
$Cs_2^{2+}(G-H)^-$	339.8318	339.8351	-9.7107	-3.3000
$(Cs_2I)^+$	392.7120	392.7154	-8.5982	-3.3766
$(Cs_3I_2)^+$	652.5204	652.5253	-7.5394	-4.9196
$(Cs_3I_2)^+G$	727.5537	727.5573	-5.0033	-3.6402
$(Cs_4I_2)^+(G-H)^-$	859.4524	859.4550	-2.9646	-2.5479
$(Cs_4I_3)^+$	912.3252	912.3352	-10.9533	-9.9929
$(Cs_5I_3)^+(G-H)^-$	1119.2674	1119.2649	2.2191	2.4837
$(Cs_5I_4)^+$	1172.1370	1172.1452	-6.9744	-8.1749

Table S3: Identified complexes in ESI of CsI with GG.

Ion	m_{meas} (Da)	m_{exact} (Da)	Δm (ppm)	Δm (Da)
Cs^+GG	264.9559	264.9589	-11.3226	-3.0000
$(Cs_2I)^+$	392.7127	392.7154	-6.9287	-2.7210
$Cs_2^{2+}(GG-H)^-$	396.8537	396.8566	-7.1512	-2.8380
$Cs^+(GG)_2$	397.0097	397.0124	-6.8966	-2.7380
$(Cs_2I)^+GG$	524.7662	524.7689	-5.0213	-2.6350
$Cs_2^{2+}(GG)(GG-H)^-$	528.9072	528.9101	-5.5000	-2.9090
$(Cs_3I_2)^+$	652.5228	652.5253	-3.7853	-2.4700
$(Cs_3I)^{2+}(GG-H)^-$	656.6639	656.6665	-3.9609	-2.6010
$(Cs_2I)^+(GG)_2$	656.8202	656.8224	-3.3434	-2.1960
$(Cs_3I_2)^+GG$	784.5755	784.5788	-4.2086	-3.3020
$(Cs_3I)^{2+}(GG)(GG-H)^-$	788.7183	788.7200	-2.0920	-1.6500
$(Cs_4I_3)^+$	912.3338	912.3352	-1.5597	-1.4230
$(Cs_4I_2)^{2+}(GG-H)^-$	916.4777	916.4764	1.4054	1.2880
$(Cs_3I_2)^+(GG)_2$	916.6303	916.6323	-2.1208	-1.9440

Table S4: Identified complexes in ESI of CsI with GGG.

Ion	m_{meas} (Da)	m_{exact} (Da)	Δm (ppm)	Δm (Da)
Cs^+GGG	321.9801	321.9804	-0.9121	-0.2937
$(Cs_2I)^+$	392.7144	392.7154	-2.4947	-0.9797
$Cs_2^{2+}(GGG-H)^-$	453.8767	453.8780	-2.9884	-1.3564
$Cs^+(GGG)_2$	511.0538	511.0554	-2.9648	-1.5152
$(Cs_2I)^+GGG$	581.7881	581.7903	-3.7647	-2.1902
$Cs_2^{2+}(GGG)(GGG-H)^-$	642.9503	642.9530	-4.2337	-2.7220
$(Cs_3I_2)^+$	652.5224	652.5253	-4.3711	-2.8522
$(Cs_3I)^{2+}(GGG-H)^-$	713.6848	713.6880	-4.3885	-3.1320
$(Cs_2I)^+(GGG)_2$	770.8626	770.8653	-3.4988	-2.6971
$(Cs_3I_2)^+GGG$	841.5980	841.6003	-2.7026	-2.2745
$(Cs_3I)^{2+}(GGG)(GGG-H)^-$	902.7605	902.7629	-2.7225	-2.4578
$(Cs_4I_3)^+$	912.3313	912.3352	-4.3088	-3.9311
$(Cs_4I_2)^+(GGG-H)^-$	973.4934	973.4979	-4.6082	-4.4860
$(Cs_3I_2)^+(GGG)_2$	1030.6706	1030.6752	-4.4420	-4.5782
$(Cs_4I_3)^+GGG$	1101.4076	1101.4102	-2.3809	-2.6224
$(Cs_5I_4)^+$	1172.1350	1172.1452	-8.6287	-10.1140
$(Cs_5I_3)^{2+}(GGG-H)^-$	1233.3025	1233.3078	-4.3312	-5.3416

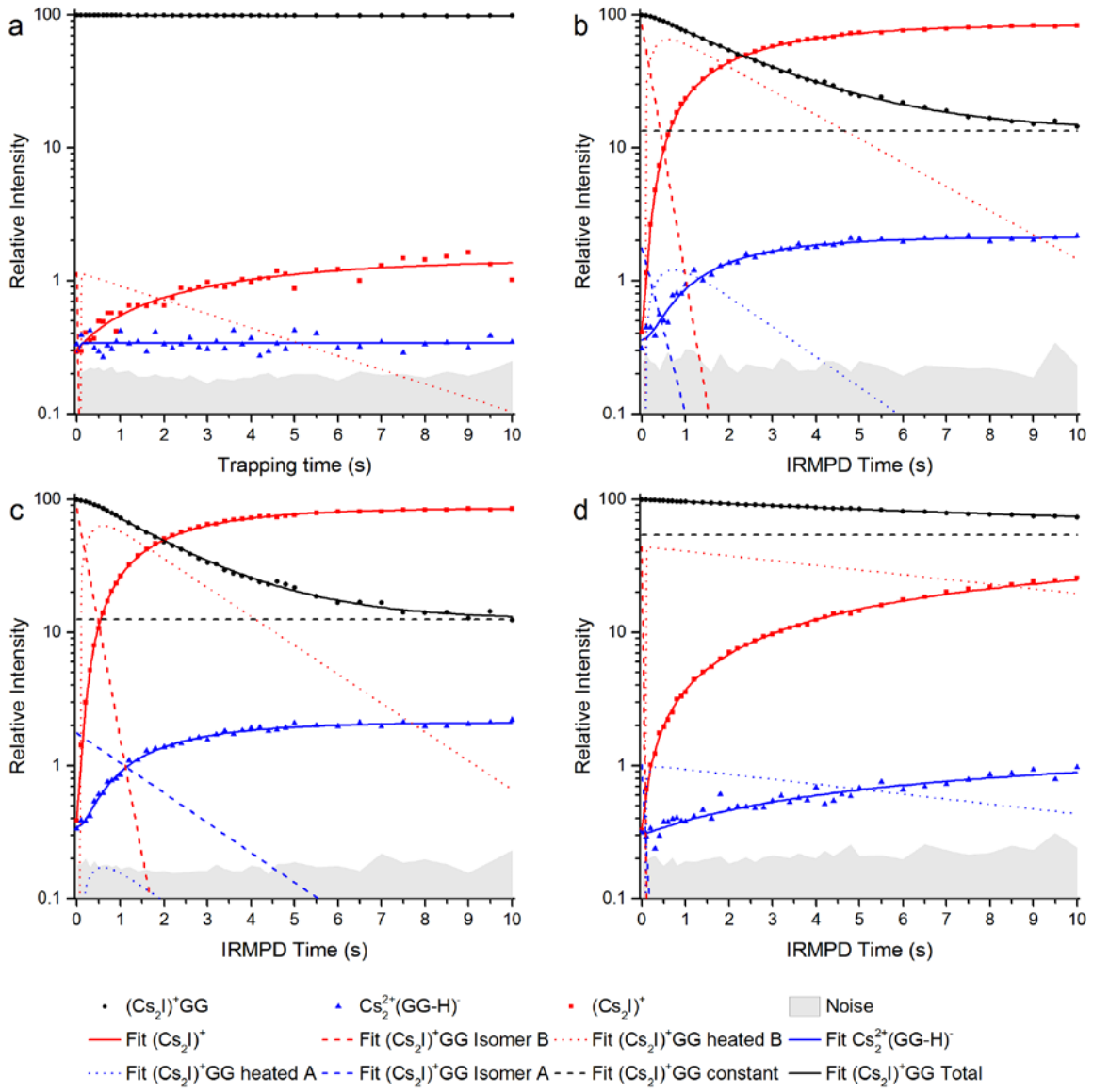

Figure S4: Kinetics of $(Cs_2I)^+GG$ at (a) without laser irradiation, i.e. fragment formation exclusively due to BIRD, (b) 2941 cm^{-1}, (c) 3390 cm^{-1} and (d) 3571 cm^{-1}. Solid lines are fits to the experimental data, the dashed lines represent the cold fraction of the respective isomer, the dotted lines the hot fraction.

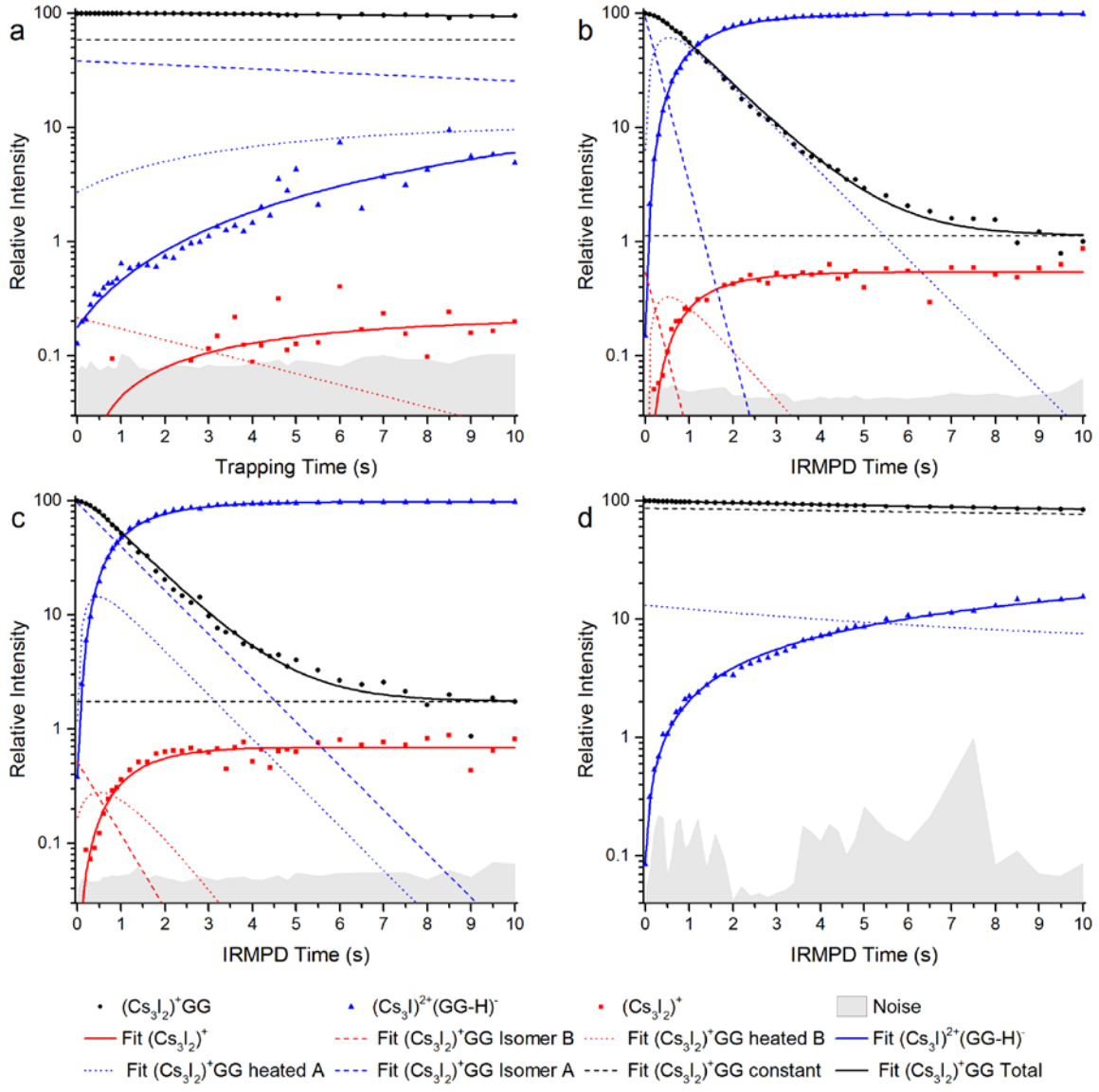

Figure S5: Kinetics of $(Cs_3I_2)^+GG$ at (a) without laser irradiation, i.e. fragment formation exclusively due to BIRD, (b) 2941 cm^{-1}, (c) 3390 cm^{-1} and (d) 3571 cm^{-1}. Solid lines are fits to the experimental data, the dashed lines represent the cold fraction of the respective isomer, the dotted lines the hot fraction.

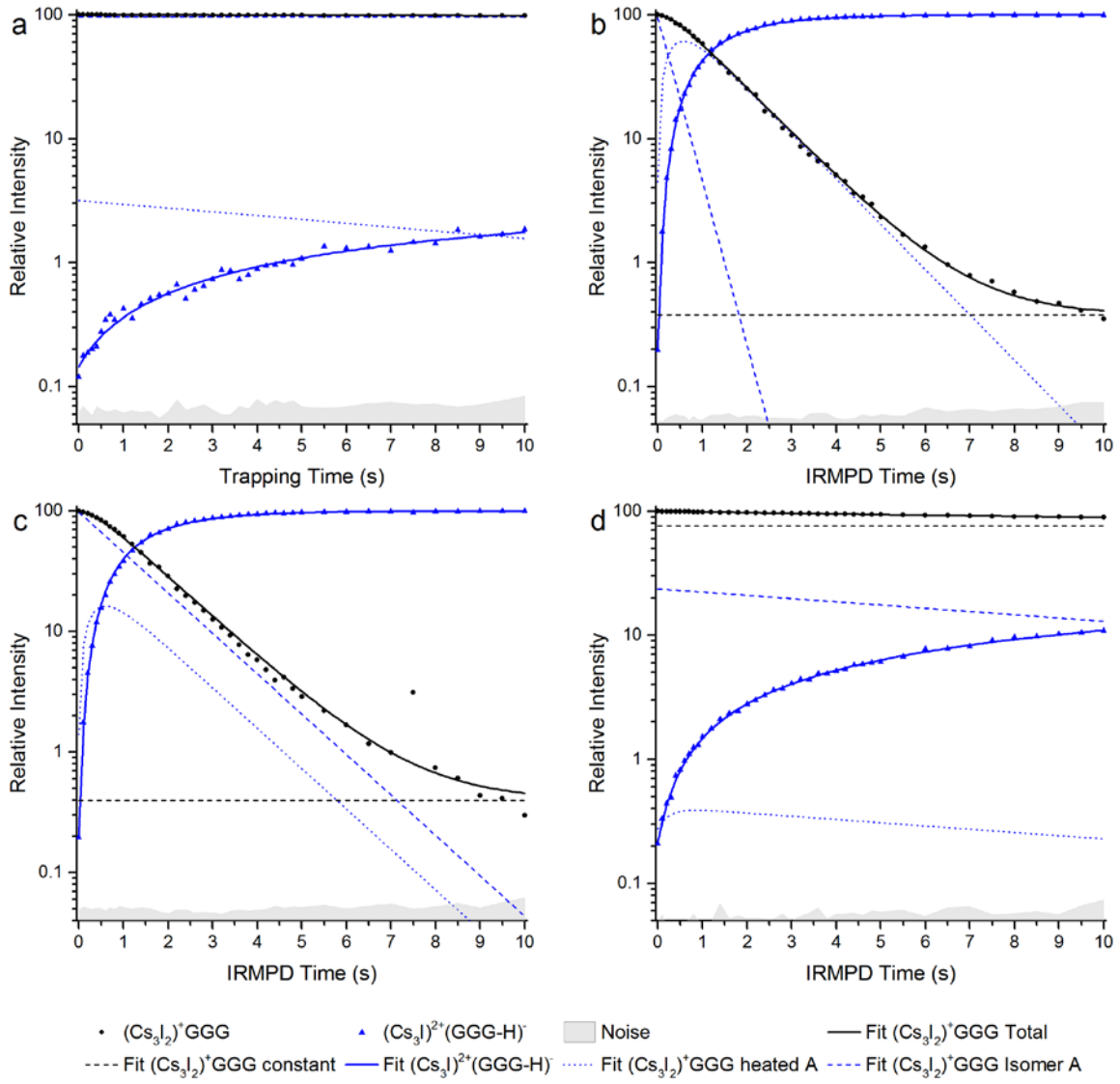

Figure S6: Kinetics of $(Cs_3I_2)^+GGG$ at (a) without radiation, (b) 2941 cm^{-1}, (c) 3390 cm^{-1} and (d) 3571 cm^{-1}. Solid lines are fits to the experimental data, the dashed lines represent the cold fraction of the ion population, the dotted lines the hot fraction.

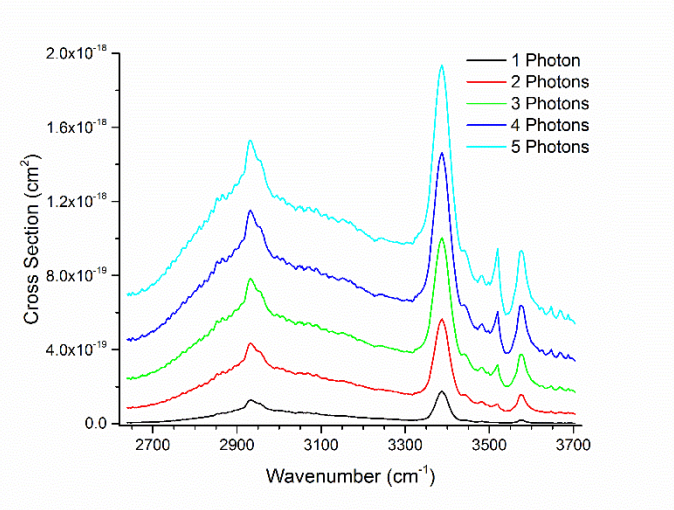

Figure S7: Absorption cross section of $(Cs_2I)^+GG$ derived for IRMPD with 1-5 photons.

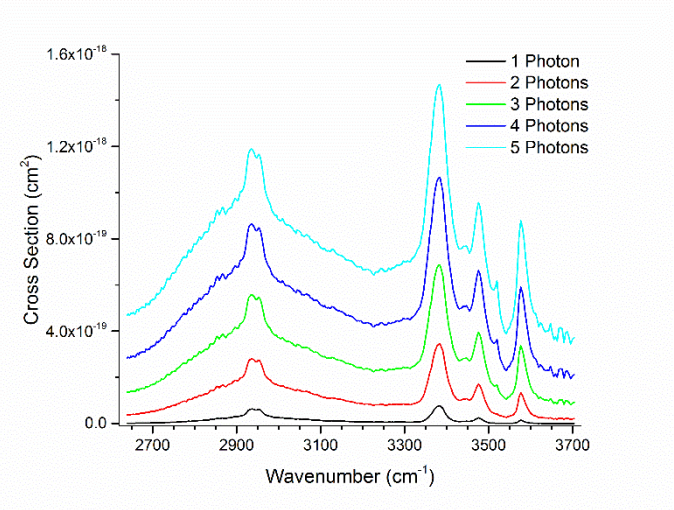

Figure S8: Absorption cross section of $(Cs_2I)^+GGG$ derived for IRMPD with 1-5 photons.

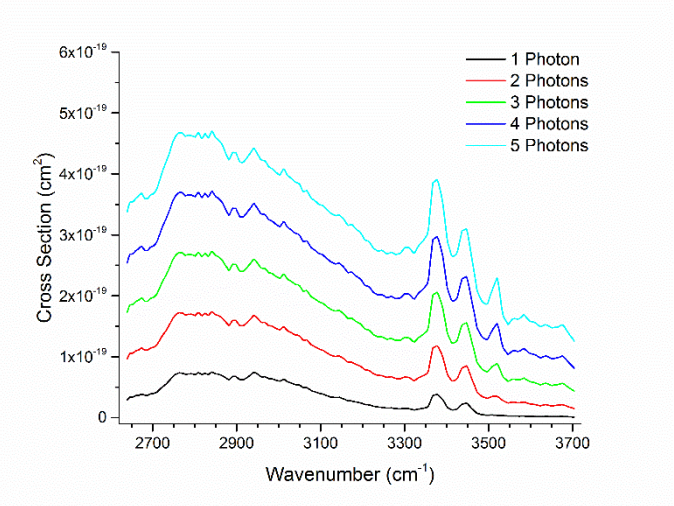

Figure S9: Absorption cross section of $(Cs_3I_2)^+G$ derived for IRMPD with 1-5 photons.

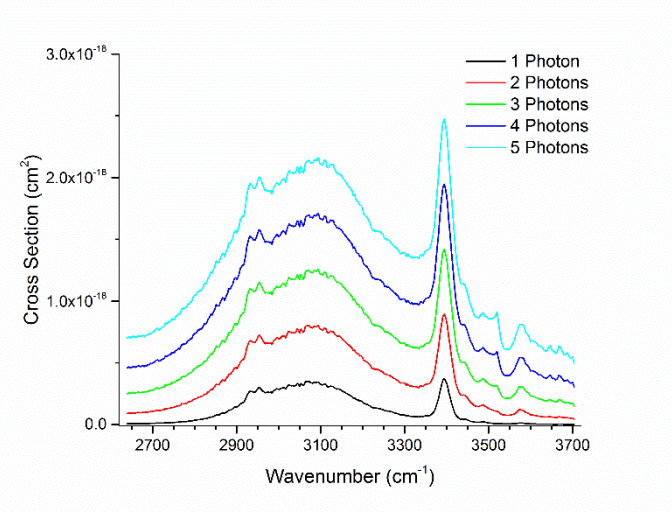

Figure S10: Absorption cross section of $(Cs_3I_2)^+GG$ derived for IRMPD with 1-5 photons.

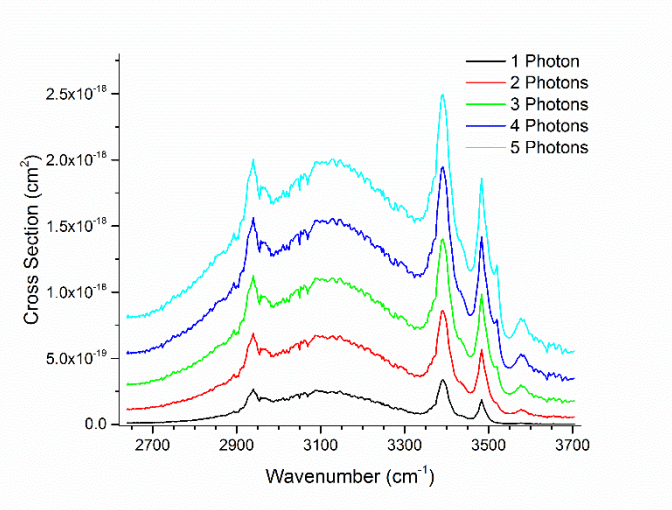

Figure S11: Absorption cross section of $(Cs_3I_2)^+GGG$ derived for IRMPD with 1-5 photons.

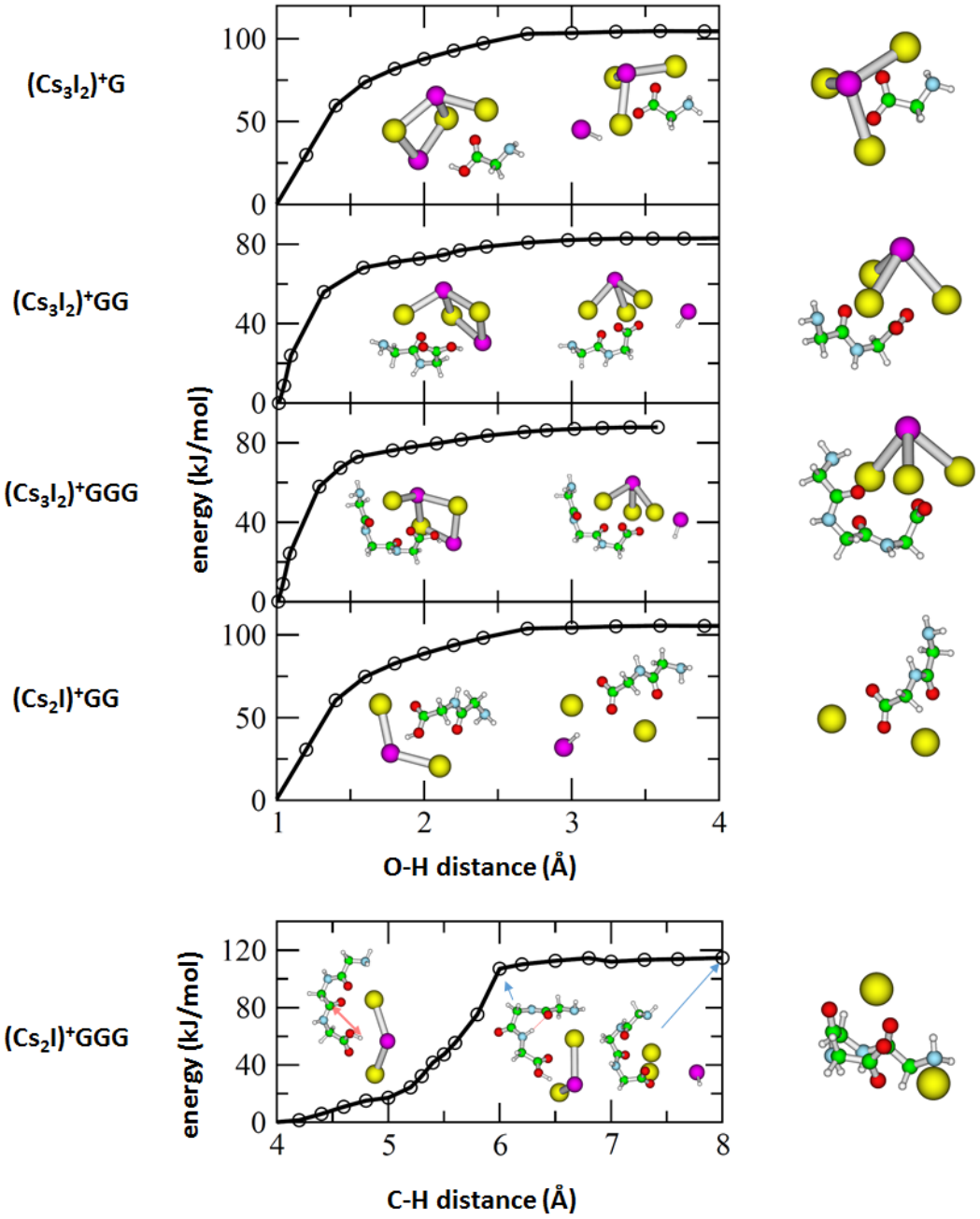

Figure S12: Relaxed scans of HI formation and dissociation from isomers **I** of the respective ions (isomer **II** for $(Cs_2I)^+$GGG), calculated at the B3LYP/def2TZVP level of theory. The O-H coordinate is used with the exception of $(Cs_2I)^+$GGG where a C-H coordinate (red arrow) is used to avoid proton transfer between oxygen atoms. For Cs_2I^+.GG, direct dissociation was possible from the initial structure. For other isomers, reorganization either of the initial structure or during the dissociation process was observed, increasing the dissociation barrier. For $(Cs_2I)^+$GGG, the break in the curve is induced by geometry relaxation, indicating a possible further small barrier (see structures). On the right hand side, the most stable calculated structures after HI elimination are shown, which correspond to the product channels of Table 1.

Cartesian coordinates of optimized clusters (in Ånsgtrom) along with the zero-point corrected energy calculated at the MP2/def2SVP+ECP(Cs,I) level of theory (in Hartree)

Cs3I2+.G, iso I
E=-306.349507
I 1.810526 -2.091729 -0.168601
Cs -1.224023 -1.036742 -2.415344
I -0.379859 2.183697 0.205633
Cs 3.486516 1.452694 -0.122881
Cs -0.895823 -1.205241 2.531080
N -4.186145 2.636501 -0.196357
C -4.126993 1.535376 0.750232
C -3.583554 0.315645 0.017330
H -3.503193 1.716658 1.635019
H -5.139096 1.275323 1.093132
O -3.133658 -0.678524 0.553837
O -3.681283 0.446687 -1.300315
H -3.309000 3.160246 -0.174800
H -4.006549 1.398310 -1.382250
H -4.948494 3.279152 0.000128

Cs3I2+.G, iso II
E=-306.342093
C 2.641107 2.335325 -2.385494
H -0.521689 1.877942 -1.907136
N 3.789497 2.108513 -1.510932
C 1.348501 2.196611 -1.608666
O 1.296245 2.362110 -0.399867
O 0.337927 1.923143 -2.401624
Cs -2.841544 -2.379781 -0.599261
I 0.644694 -1.751915 1.164475
Cs -0.477224 2.020813 2.041504
Cs 4.036158 -0.963038 -0.423555
I -2.832900 1.458528 -0.946745
H 4.616158 2.498379 -1.962203
H 3.644027 2.691481 -0.685324
H 2.629719 1.618520 -3.216384
H 2.612809 3.340294 -2.843068

Cs3I2+.G, iso III
E=-306.340319
C 5.786550 -1.777041 0.809177
N 6.262359 -1.108978 -0.392112
C 4.496829 -2.512363 0.472477
O 3.717763 -2.954914 1.290824
O 4.298118 -2.622064 -0.840300
Cs -5.935764 -0.933031 0.049839
I -2.271703 0.072229 -0.044588
Cs 1.195922 -2.093136 -0.174105
I 3.285300 1.245121 -0.093657
Cs 0.127041 3.303616 0.088824
H 7.275662 -1.046175 -0.422811
H 5.070100 -2.102887 -1.213593
H 5.582216 -1.117269 1.663573
H 6.510581 -2.535747 1.138523
H 5.881040 -0.162112 -0.438652

Cs3I2+.G, iso IV
E=-306.339629
I -1.386461 0.542671 2.249722
Cs -3.828058 -0.211781 -0.744517
I -0.195618 -0.495418 -2.250652
Cs 1.128732 -2.291972 1.203531
Cs 1.044111 2.605141 -0.065576
C 4.595899 -0.996248 -1.113777
C 4.557520 0.268596 -0.295683
O 5.787569 0.707169 -0.030042
O 3.547182 0.851250 0.052653
H 5.711619 1.543005 0.458198
N 3.319189 -1.687181 -1.098023
H 2.611818 -1.099768 -1.548050
H 3.395523 -2.490493 -1.721285
H 4.947963 -0.689272 -2.116440
H 5.387238 -1.635388 -0.700191

Cs3I2+.G, iso V
E=-306.339054
C 9.230845 0.203182 0.051025
N 9.744637 -1.160091 0.110391
C 7.705551 0.168970 0.022121
O 7.003667 1.156819 -0.028614
O 7.211370 -1.065174 0.058775
Cs 4.120374 0.283329 -0.044544
I 0.289423 0.061861 -0.016420
Cs -2.776207 2.704528 0.012222
I -5.255492 -0.128757 0.021279
Cs -2.582604 -2.779213 -0.006495
H 10.303123 -1.323711 0.944131
H 8.037896 -1.628543 0.095837
H 9.563253 0.749014 -0.842263
H 9.528255 0.811741 0.915658
H 10.332019 -1.383852 -0.688818

Cs3I2+.G, iso VI
E=-306.334964
C -0.738321 -2.047266 1.890812
C -1.937802 -2.291620 1.006590
O -1.700566 -3.088456 -0.047627
N 0.372327 -2.949596 1.675218
O -3.027309 -1.787157 1.197998
Cs -4.501336 0.721533 0.565590
I -1.082214 0.968133 -1.243419
Cs 2.158685 2.992673 -0.070960
I 3.210133 -0.398340 1.273749
Cs 1.271825 -2.478589 -1.370919
H 1.223634 -2.499986 2.017937
H 0.250158 -3.799773 2.220782
H -0.413897 -1.024647 1.641097
H -1.126933 -2.001456 2.922161
H -2.543807 -3.146660 -0.527526

Cs3I2+.GG, iso I
E=-513.579328

C -4.802684 -1.664197 0.350349
N -5.333169 -0.328100 0.451022
C -3.365922 -1.753841 0.842755
O -2.554304 -2.518321 0.358846
O -3.139100 -0.938886 1.859917
Cs 0.176807 -2.988585 -0.667898
I 2.080586 0.129292 -2.181514
Cs 3.956082 0.879902 1.163983
I 0.280506 -0.039176 2.205500
Cs -1.199308 2.091424 -1.072076
C -4.644263 0.677811 -0.131924
H -6.050358 -0.120788 1.132833
H -4.809826 -2.018328 -0.687611
H -5.422398 -2.343181 0.950366
H -2.179677 -0.935426 2.085364
C -5.156700 2.085379 0.118185
O -3.655235 0.453661 -0.828027
N -4.049149 2.953601 0.508519
H -5.570384 2.444342 -0.835293
H -5.990902 2.064104 0.840387
H -4.381811 3.916510 0.528102
H -3.796748 2.744829 1.475233

Cs3I2+.GG, iso II
E=-513.574443
C 1.011718 0.306597 2.364387
N 1.767742 1.488518 2.765224
C 1.946048 -0.809616 1.927216
N 1.400394 -2.044421 1.929806
O 3.119427 -0.615609 1.600161
I -2.289470 -1.858089 1.210856
Cs -0.420031 -1.867222 -2.210255
I -0.117570 2.001501 -1.376559
Cs 3.531038 2.031217 0.165774
Cs -3.596153 1.733801 0.532945
H 1.106887 2.203210 3.064989
H 2.309168 1.262537 3.599344
H 0.381002 0.559538 1.499121
H 0.336348 -0.091069 3.139116
C 2.221510 -3.168363 1.592100
H 0.390806 -2.153177 2.035486
C 2.663474 -3.184598 0.143665
H 3.124497 -3.195234 2.215448
H 1.661740 -4.095397 1.778170
O 3.769548 -3.913005 -0.005272
O 2.078101 -2.658624 -0.781223
H 3.975684 -3.944942 -0.953712

Cs3I2+.GG, iso III
E= -513.573638
C -1.306361 1.082098 -2.272321
H 0.586672 1.345007 -2.100413
I 2.280728 2.357579 -0.565332
I 0.482099 -2.327631 1.127329
Cs -2.962719 -1.901573 -0.592403
Cs 3.634826 -1.314976 -0.953319
Cs 0.015421 1.324700 2.485128
O -0.059715 0.717581 -2.509920
O -2.245525 0.336711 -2.471282
C -1.503400 2.507035 -1.754359
N -2.829613 2.671370 -1.222919
C -3.205676 1.940926 -0.148978
C -4.701800 1.833199 0.072581
N -5.168384 0.618210 -0.604823
H -1.342460 3.212500 -2.580233
H -0.737176 2.725789 -1.000871
H -3.546883 3.057121 -1.823617
O -2.390421 1.341367 0.555596
H -5.204943 2.757923 -0.260266
H -4.870527 1.729082 1.150843
H -6.161336 0.496068 -0.408364
H -5.112532 0.769118 -1.612768

Cs3I2+.GG, iso IV
E=-513.572128
C -3.871628 -0.602329 1.692908
N -4.159821 0.774973 1.388426
C -4.172499 -1.543421 0.548369
O -3.450108 -2.470974 0.240587
O -5.348583 -1.299308 -0.021801
Cs -0.472323 -2.850963 0.265492
I 2.228377 -0.971648 -1.875982
Cs -0.700199 1.655758 -2.147658
I -0.016407 0.909185 1.983581
Cs 3.851242 0.733487 1.252320
H -2.814284 -0.725541 1.962801
H -4.491787 -0.912991 2.544582
C -3.626972 1.337905 0.280860
H -5.467294 -1.958893 -0.725435
H -4.494477 1.371726 2.133032
C -3.774366 2.846220 0.176927
O -3.074392 0.661992 -0.586549
N -2.478584 3.445375 -0.126192
H -4.470446 3.047694 -0.650834
H -4.246091 3.237201 1.094783
H -2.595272 4.456279 -0.178481
H -1.858069 3.283140 0.670444

Cs3I2+.GG, iso V
E=-513.571658
C 3.881317 -0.322678 -3.084956
N 4.420548 -1.558758 -2.574136
C 3.457753 0.622915 -1.967394
O 2.555149 1.427629 -2.096536
O 4.201798 0.465992 -0.886405
Cs 0.950689 -2.022222 1.009302
I 2.614327 1.380162 2.056320
Cs 0.317219 2.832852 -0.702767
I -2.430405 -0.070160 -0.203652
Cs -6.172143 -0.575083 -0.119211
C 3.647143 -2.272373 -1.720953
H 5.424569 -1.673987 -2.533396
H 2.997157 -0.506255 -3.706153
H 4.639224 0.174616 -3.704178
H 3.820412 0.967852 -0.119942
C 4.327153 -3.406317 -0.974019

O 2.460960 -2.000090 -1.552739
N 4.038015 -3.280742 0.451913
H 3.890799 -4.344861 -1.345201
H 5.403095 -3.432947 -1.219655
H 4.422244 -4.089592 0.937747
H 4.554168 -2.480931 0.821530

Cs3I2+.GG, iso VI
E=-513.571533
C 4.071192 0.824011 -1.662100
N 3.461670 -0.466177 -1.412935
C 3.889349 -1.427307 -0.563135
O 3.158031 -2.336910 -0.165485
C 3.496967 1.876952 -0.715666
O 2.875649 2.842042 -1.104012
O 3.633800 1.624016 0.588913
C 5.323501 -1.334574 -0.065400
N 5.360634 -0.385649 1.057126
Cs 0.578123 2.756446 0.936783
I -0.190388 -0.045653 -2.126091
Cs 0.362380 -2.952394 0.611737
I -1.912867 -0.085310 2.221486
Cs -3.977679 0.164536 -1.120758
H 5.160776 0.769560 -1.548209
H 3.850581 1.143593 -2.686239
H 2.473937 -0.533785 -1.682006
H 5.631522 -2.350977 0.214855
H 5.998439 -0.981096 -0.853702
H 6.323355 -0.139092 1.287929
H 4.311643 0.894777 0.766594
H 4.984937 -0.839232 1.891080

Cs3I2+.GG, iso VII
E=-513.564704
C -3.873248 1.573774 0.117090
C -3.300793 0.159894 0.359788
O -3.049509 -0.100638 1.561442
N -3.229235 2.472343 1.057266
C -2.607598 3.586546 0.682653
O -2.655257 4.118395 -0.430205
O -3.140894 -0.576496 -0.645445
C -1.764997 4.283406 1.759772
N -0.807188 5.111529 0.998344
Cs -0.834193 0.178573 -2.327908
I 1.414093 2.648257 0.120214
Cs 3.995093 -0.261451 0.712596
I 1.221939 -2.644224 -0.469515
Cs -2.331692 -2.976226 1.148592
H -2.979597 1.996349 1.925092
H -3.686590 1.929694 -0.901122
H -4.962024 1.557432 0.275425
H -2.399061 4.930272 2.378573
H -1.216235 3.578316 2.393441
H 0.010382 4.511708 0.711503
H -1.311895 5.351895 0.119369
H -0.471135 5.942423 1.488886

Cs3I2+.GGG, iso I
E=-720.816465
C 2.537602 3.350288 0.381300
C 3.456782 2.178959 0.084432
O 3.464306 1.564657 -0.979174
N 1.858947 3.818154 -0.814199
N 4.277553 1.803115 1.099380
C 5.079380 0.623977 0.921369
C 4.214731 -0.611401 0.703670
N 4.694273 -1.523822 -0.167255
O 3.180406 -0.805660 1.341515
I -1.185038 2.011679 1.305556
Cs -4.488017 0.365501 0.004635
I -1.690028 -2.100274 -1.141925
Cs 0.803556 1.041556 -2.280940
Cs 0.453895 -1.467418 2.274395
H 1.074906 4.401176 -0.526608
H 2.481470 4.422096 -1.348091
H 1.773601 2.984859 1.084213
H 3.119422 4.122690 0.916741
H 4.228140 2.258411 2.000617
H 5.772057 0.753687 0.077515
H 5.678124 0.458670 1.827124
C 3.927652 -2.719872 -0.402650
H 5.411826 -1.250231 -0.825778
C 2.555866 -2.395344 -0.973613
H 4.458861 -3.355648 -1.122858
H 3.808651 -3.291603 0.525444
O 1.626046 -3.237166 -0.530188
O 2.359490 -1.484979 -1.747987
H 0.763053 -3.025308 -0.961546

Cs3I2+.GGG, iso II
E=-720.809601
C 2.007976 3.862566 -0.161211
N 2.985973 3.484765 0.825799
C 3.606884 2.287350 0.732958
C 4.427852 1.886196 1.957925
N 5.461446 0.947063 1.622616
C 5.163915 -0.365371 1.446359
O 4.068473 -0.844645 1.718639
C 0.665495 3.161420 -0.015953
O -0.116059 3.081439 -0.944658
O 0.466936 2.713378 1.208714
O 3.514999 1.562983 -0.254780
C 6.294079 -1.233874 0.918833
N 5.719516 -2.374120 0.216216
Cs -2.519797 1.739816 -2.075012
I -2.737413 1.392280 1.821284
Cs -2.977721 -2.441793 1.679918
I -0.959776 -1.911723 -1.654287
Cs 2.826239 -1.277417 -1.086533
H 2.968057 3.953800 1.723164
H 2.391626 3.644011 -1.163358
H 1.827550 4.944427 -0.101226
H -0.445558 2.332209 1.303992
H 4.867645 2.768239 2.441694
H 3.740310 1.411060 2.672037
H 6.324664 1.304233 1.233939

H 6.936733 -1.499159 1.778811
H 6.917707 -0.654950 0.223124
H 6.473998 -2.964343 -0.129772
H 5.228069 -2.941292 0.907030

Cs3I2+.GGG, iso III
E=-720.801964
C 6.441766 -1.620183 -0.341911
N 6.017133 -0.338421 0.154885
C 4.760606 0.110521 -0.003317
O 3.885948 -0.528346 -0.587422
C 7.920467 -1.774648 -0.065564
O 8.372249 -2.948518 -0.505629
O 8.590947 -0.932894 0.485958
C 4.466600 1.464679 0.634417
N 3.737679 2.340317 -0.245577
Cs 1.042293 -1.322731 -0.429232
I -1.950154 -1.334802 2.181287
Cs -1.145009 2.474827 1.514175
I -1.888205 0.727730 -2.206293
Cs -4.639515 -1.581688 -0.641770
H 5.900553 -2.448343 0.140042
H 6.264136 -1.714179 -1.423446
H 9.321614 -2.990699 -0.300680
H 6.732290 0.219736 0.612713
H 3.841966 1.279901 1.518976
H 5.387505 1.961655 0.967265
C 2.383211 2.415202 -0.255618
H 4.258598 2.890909 -0.916894
C 1.826232 3.416486 -1.260103
O 1.674551 1.737009 0.486495
H 2.341435 4.373509 -1.089041
H 2.136997 3.072490 -2.265119
N 0.396768 3.604414 -1.105101
H 0.119566 4.407028 -1.667685
H -0.092832 2.815855 -1.537395

Cs3I2+.GGG, iso IV
E=-720.801928
C 3.566154 -0.822571 2.989382
C 2.921868 -1.531772 1.807450
O 3.623477 -1.411175 0.698704
N 4.458144 0.246879 2.624326
C 3.974311 1.302767 1.931258
O 2.776994 1.447589 1.703326
O 1.883063 -2.154168 1.932531
C 5.024636 2.301868 1.445702
N 4.427628 3.549161 1.058710
Cs 1.104939 1.354266 -0.949145
I -2.595969 0.125153 0.398992
Cs -6.130179 1.400600 0.116972
I 1.844625 -2.339587 -2.133301
Cs -0.566658 -3.319749 0.694174
H 5.457353 0.089638 2.652771
H 2.748596 -0.446716 3.616779
H 4.119907 -1.568803 3.574054
H 3.149559 -1.840006 -0.065806
H 5.782725 2.473472 2.221624
H 5.523312 1.865041 0.569238
H 4.156479 4.189256 1.794124
C 3.773070 3.629931 -0.130683
C 2.972219 4.900351 -0.362442
O 3.849859 2.761160 -0.990645
H 3.691446 5.698713 -0.625042
N 1.957246 4.637983 -1.372881
H 2.485248 5.206441 0.574581
H 1.456742 5.501580 -1.573359
H 2.442425 4.396038 -2.236971

Cs3I2+.GGG, iso V
E=-720.801799
C 3.522744 0.954285 -1.491221
C 4.155887 -0.323593 -0.979416
O 5.083275 -0.305995 -0.174342
N 3.650375 1.961631 -0.467599
C 2.881088 3.067191 -0.458024
O 1.999964 3.275911 -1.291921
N 3.667722 -1.468824 -1.507845
C 3.145586 4.056851 0.666251
N 1.950600 4.862553 0.881474
I -0.101680 -0.967310 -1.863674
Cs -3.910950 -1.667356 -1.145454
I -2.637639 0.456046 1.895963
Cs -0.799949 3.081458 -0.422619
Cs 0.774593 -1.510944 2.039588
H 2.465014 0.802939 -1.739171
H 4.038604 1.244518 -2.422303
H 4.422355 1.839336 0.181811
H 3.386891 3.508590 1.587540
H 4.048797 4.636035 0.397482
H 2.109010 5.484602 1.672141
H 1.843017 5.475952 0.074341
C 4.305596 -2.702781 -1.154678
H 2.760913 -1.466454 -1.970788
C 4.184874 -3.036403 0.319399
H 3.851862 -3.525596 -1.723680
H 5.374729 -2.676492 -1.401858
O 5.150697 -3.871260 0.694126
O 3.304996 -2.648300 1.061167
H 5.012525 -4.083725 1.631537

Cs3I2+.GGG, iso VI
E=-720.800678
C -4.731131 0.659784 0.560753
C -3.311004 0.429164 1.136766
O -2.523849 1.423316 1.093540
N -4.683631 1.598231 -0.540982
C -3.818469 1.308012 -1.546409
C -3.157638 2.525946 -2.166346
N -2.374593 3.101275 -1.078921
C -1.399284 3.978512 -1.311192
O -1.067916 4.443823 -2.402110
O -3.487033 0.158342 -1.822581
O -3.058980 -0.706356 1.590300
C -0.665819 4.473265 -0.059274
N 0.633861 4.983500 -0.543834

Cs -0.205002 -0.063487 2.500290
I 2.482044 2.274874 0.443680
Cs 4.193192 -0.932937 -1.085505
I 1.018338 -2.829805 -0.076462
Cs -2.785715 -2.581317 -0.801729
H -5.380392 1.065771 1.347272
H -5.164381 -0.293189 0.237559
H -4.785619 2.577632 -0.304424
H -2.514811 2.213171 -2.997764
H -3.895363 3.249889 -2.546809
H -2.421618 2.598723 -0.163110
H -1.236880 5.288095 0.401629
H -0.493390 3.678170 0.673818
H 0.961100 5.825145 -0.064952
H 1.362916 4.233416 -0.417737
H 0.484903 5.168128 -1.558983

Cs2I+.GG, iso I
E=-502.100415
C -4.170797 2.037708 0.648915
C -2.811168 2.226847 -0.006758
N -2.046957 3.214211 0.520712
C -0.693939 3.385534 0.066274
C 0.236392 2.220897 0.373119
O 1.360181 2.167846 -0.091357
N -4.851039 0.880997 0.083310
O -2.438500 1.547239 -0.958534
O -0.298522 1.320205 1.179036
Cs -2.612658 -1.477376 -0.501391
I 1.070322 -1.820522 0.644848
Cs 3.881168 0.561012 -0.406736
H -5.752225 0.777854 0.547225
H -5.075974 1.094805 -0.888362
H -4.724653 2.989339 0.553075
H -4.013690 1.874260 1.725686
H -2.333218 3.651452 1.387094
H -0.669048 3.519857 -1.023014
H -0.267757 4.291572 0.515394
H 0.279209 0.513846 1.202281

Cs2I+.GG, iso II
E=-502.099793
H -0.231124 1.680213 -0.053743
I 1.683662 -0.289621 0.011436
Cs 5.355368 0.490371 0.036277
O -0.978667 2.189669 -0.434770
C -2.114506 1.786572 0.124889
O -2.198541 0.980485 1.026583
Cs -1.891938 -1.861120 -0.030578
C -3.300625 2.447555 -0.556882
H -3.171702 2.298774 -1.639137
H -3.254717 3.528524 -0.373533
N -4.558198 1.931759 -0.108652
H -5.234540 2.492796 0.403974
C -4.903299 0.646871 -0.296670
O -4.190479 -0.184962 -0.862672
C -6.261020 0.277857 0.286793
H -6.051130 -0.290528 1.204832
H -6.727820 -0.427322 -0.420406
N -7.056999 1.446072 0.620240
H -7.618342 1.737101 -0.176943
H -7.708728 1.242116 1.372427

Cs2I+.GG, iso III
E=-502.095797
Cs -1.636364 0.406086 -0.003889
I 2.140008 0.064486 -0.024912
Cs 5.852641 -0.189995 0.016637
N -3.904804 2.861753 -0.117540
H -3.842182 3.023684 0.887453
H -3.897000 3.787393 -0.541818
C -5.188264 2.227452 -0.382839
H -6.064808 2.772775 0.014206
H -5.334784 2.141978 -1.468955
C -5.193827 0.845254 0.245896
O -4.491715 0.575912 1.215101
N -6.037262 -0.059211 -0.310609
H -6.505243 0.159693 -1.179916
C -6.056363 -1.408658 0.175393
H -6.150140 -1.420406 1.270314
H -6.920503 -1.947653 -0.231622
C -4.789836 -2.170554 -0.173692
O -3.809837 -1.694262 -0.704039
O -4.894904 -3.444815 0.202466
H -4.065230 -3.893673 -0.030232

Cs2I+.GG, iso IV
E=-502.094126
I 0.103885 -1.582818 0.867126
Cs -3.478096 -0.743432 -0.366439
Cs 3.466052 -0.726925 -0.727433
C -1.545112 2.163478 -0.882368
O -1.814538 1.872353 0.389314
O -2.253419 1.748983 -1.776070
C -0.346578 3.064318 -1.188620
H 0.309783 2.527735 -1.882695
H -0.724715 3.949609 -1.716724
N 0.404978 3.428471 -0.017113
H -0.099739 3.969534 0.675709
C 1.378919 2.603523 0.471276
O 2.069577 1.880717 -0.236956
C 1.390076 2.550202 1.989143
H 1.426326 3.568085 2.403138
H 2.284510 2.008404 2.327208
N 0.120502 1.914852 2.358922
H 0.204085 0.897009 2.251229
H -0.105698 2.086512 3.337586
H -1.093206 2.043284 1.070276

Cs2I+.GG, iso V
E=-502.092955
I -0.071677 -1.889596 0.013713
Cs -3.552527 -0.271288 -0.639770
Cs 3.526125 -0.831821 0.033099
N -2.225589 0.292505 2.262399
H -2.575132 0.028597 3.181444

H -1.611075 -0.471548 1.969639
C -1.419292 1.490687 2.399530
H -2.003252 2.263791 2.923410
H -0.492553 1.348531 2.985084
C -1.058702 2.091200 1.047412
O -1.786958 2.023367 0.065532
N 0.116939 2.782122 1.044243
H 0.700383 2.760218 1.869580
C 0.567562 3.505759 -0.104647
H -0.224180 3.459391 -0.863344
H 0.737510 4.571154 0.114945
C 1.836849 2.958114 -0.718929
O 2.490118 2.023330 -0.301896
O 2.163037 3.671447 -1.797350
H 2.991711 3.317318 -2.157642

Cs2I+.GG, iso VI
E=-502.090942
I -1.401431 -2.064749 -0.109534
Cs 2.459086 -1.781092 -0.078534
Cs -3.345484 1.207580 -0.332233
O 0.426097 0.048462 1.907271
H -0.308280 -0.479726 1.493158
C 0.314735 1.317825 1.545876
O -0.599694 1.780683 0.891274
C 1.463061 2.164458 2.072529
H 2.235561 1.509349 2.494087
H 1.074406 2.800400 2.877988
N 2.001764 3.002670 1.032408
H 1.950089 4.009666 1.112174
C 2.566201 2.433506 -0.057300
O 2.616392 1.207164 -0.179363
C 3.117004 3.395870 -1.104193
H 3.847210 4.055091 -0.609691
H 2.290221 4.050315 -1.423048
N 3.721865 2.784151 -2.256830
H 3.057857 2.155905 -2.702168
H 4.506919 2.205717 -1.969042

Cs2I+.GGG, iso I
E=-709.332190
C 4.804826 0.064826 1.752782
N 5.185623 0.596892 0.456193
C 4.765995 -0.030097 -0.681272
O 4.492543 -1.219949 -0.743802
C 3.345094 0.430888 1.983589
O 3.177372 1.743614 1.900915
O 2.457109 -0.387244 2.124718
C 4.644007 0.915407 -1.884342
N 3.828367 2.061036 -1.522686
C 2.588549 1.827541 -1.023633
O 2.153995 0.683610 -0.933106
C 1.757081 3.004381 -0.550847
N 1.009370 2.574342 0.627606
Cs 1.455228 -2.057387 -0.159961
I -1.952352 -0.024328 -0.150190
Cs -5.681443 0.254034 0.072882
H 4.922119 -1.022148 1.750747
H 5.443998 0.499457 2.531795
H 5.175961 1.610005 0.415967
H 5.635121 1.270275 -2.195271
H 4.196326 0.339638 -2.704261
H 4.169763 3.005183 -1.648518
H 2.403263 3.852796 -0.286594
H 1.114588 3.319494 -1.392022
H 2.219377 1.988338 1.650994
H 0.418459 3.332913 0.964268
H 0.372508 1.814008 0.367082

Cs2I+.GGG, iso II
E=-709.332057
C 0.087666 3.254741 -0.332740
C -0.844150 2.140697 0.115871
O -0.232938 1.184051 0.790106
N 1.373190 3.305649 0.307926
C 2.388518 2.487939 -0.063503
C 3.686523 2.700919 0.723049
N 4.757165 1.895586 0.210879
C 4.732793 0.557165 0.440187
C 5.762896 -0.268731 -0.309808
N 5.302614 -1.649043 -0.382542
O 2.290478 1.660533 -0.961567
O -2.025479 2.147634 -0.180218
O 3.950885 0.042173 1.232337
Cs -4.626508 0.617940 -0.244706
Cs 1.945120 -1.484429 -0.446587
I -1.818789 -1.859537 0.486187
H -0.437222 4.208208 -0.200328
H 0.231594 3.109194 -1.413208
H 1.492154 3.904270 1.115146
H 3.972164 3.761034 0.688742
H 3.506239 2.431069 1.772666
H 5.267337 2.237112 -0.593554
H 5.882277 0.128939 -1.327679
H 6.733717 -0.131517 0.201549
H 5.992432 -2.200710 -0.889559
H 5.302378 -2.023956 0.566078
H -0.850722 0.411827 0.895914

Cs2I+.GGG, iso III
E=-709.330304
C -2.652394 2.535692 -1.171525
C -1.529437 1.892605 -0.376776
O -0.339497 2.250408 -0.827613
N -3.895638 1.832552 -1.005474
C -3.989185 0.568805 -1.501294
C -5.317004 -0.135083 -1.220184
N -5.772034 0.123006 0.124342
C -4.960458 -0.246359 1.152168
C -5.135877 0.565616 2.418348
N -4.581770 1.887433 2.120434
O -3.098219 0.044588 -2.162549
O -1.725313 1.137974 0.557963
O -4.064452 -1.073070 1.003687
Cs -1.422631 -1.810111 -0.174765
I 2.178386 -0.208185 0.088066

Cs 5.889871 0.342864 0.139962
H -2.359800 2.550519 -2.228072
H -2.770956 3.577019 -0.842838
H -4.461909 2.074260 -0.193356
H -6.071769 0.216642 -1.935455
H -5.166410 -1.208043 -1.381743
H -6.425526 0.879652 0.284927
H -6.203338 0.668053 2.660811
H -4.644906 0.025600 3.242447
H -4.764381 2.528568 2.889869
H -3.567071 1.802649 2.042680
H 0.355509 1.749704 -0.344055

Cs2I+.GGG, iso IV
E=-709.325875
C 1.306048 1.540108 -1.747781
N 0.658635 2.311860 -0.714691
C 1.090321 2.206317 0.559749
O 2.098320 1.569253 0.866768
C 2.801719 1.779356 -1.777003
O 3.631130 0.896080 -1.826309
O 3.099076 3.079375 -1.792664
C 0.247033 2.936807 1.593947
N -0.585495 2.015932 2.332150
C -1.734140 1.527459 1.804927
O -2.129463 1.846322 0.683652
C -2.523517 0.638495 2.755158
N -3.164089 -0.465098 2.060522
Cs 3.435124 -1.150805 0.422746
H 1.125843 0.464808 -1.615677
H 0.903871 1.849347 -2.721661
H -0.281341 2.658726 -0.863043
H 0.930603 3.436079 2.290499
H -0.389036 3.695826 1.121385
H -0.237025 1.631340 3.199907
H -1.862845 0.323629 3.582251
H -3.295806 1.284661 3.201031
H -2.434204 -1.122377 1.772209
H -3.743136 -0.972701 2.727219
H 4.067650 3.149033 -1.831625
I -0.329542 -1.827054 -0.108514
Cs -3.733296 -0.112883 -1.030795

Cs2I+.GGG, iso V
E=-709.325376
C 2.462654 -3.348401 0.052006
N 3.815020 -2.869752 0.128216
C 4.158967 -1.759068 -0.575088
O 3.409802 -1.262193 -1.409091
C 1.471947 -2.279274 0.495365
O 1.792990 -1.241694 1.038369
O 0.234804 -2.635695 0.186536
C 5.465639 -1.103994 -0.149952
N 5.192822 -0.233874 0.979876
C 4.673284 1.008726 0.779863
O 4.618814 1.540573 -0.322188
C 4.177758 1.720560 2.028501
N 3.222907 2.746243 1.636657
Cs 1.603403 1.244096 -0.923821
H 2.201434 -3.639787 -0.973859
H 2.343255 -4.236131 0.686068
H 4.431202 -3.225039 0.846203
H 6.229011 -1.842753 0.129114
H 5.838534 -0.493790 -0.978176
H 5.016804 -0.670812 1.876304
H 3.677854 0.993819 2.684522
H 5.064791 2.093997 2.574053
H 2.889010 3.227826 2.468982
H 3.722077 3.447577 1.090521
H -0.386390 -1.902595 0.397505
I -2.075818 0.132537 -0.035212
Cs -5.813171 -0.060720 0.198705

Cs2I+.GGG, iso VI
E=-709.324567
C 0.169414 2.630992 2.263586
N 1.027038 3.233267 1.264948
C 1.673078 2.449523 0.371890
O 1.411346 1.257860 0.247600
C -0.808334 1.649102 1.632578
O -1.584201 1.962227 0.749542
O -0.733862 0.461349 2.206261
C 2.767672 3.130780 -0.450744
N 3.296990 2.254728 -1.455760
C 4.017708 1.164635 -1.071262
O 4.378703 0.985685 0.084713
C 4.400624 0.201262 -2.181748
N 4.597801 -1.123213 -1.607084
H 0.753122 2.109254 3.034064
H -0.416779 3.424597 2.743382
H 1.307258 4.198785 1.382116
H 2.383364 4.046494 -0.920127
H 3.572833 3.418438 0.240480
H 2.864368 2.252203 -2.369923
H 3.602855 0.159910 -2.937252
H 5.292415 0.621251 -2.682981
H 4.952808 -1.748096 -2.328879
H 5.350558 -1.042871 -0.922723
H -1.267889 -0.197460 1.693741
Cs 2.116269 -1.643208 0.514698
I -1.752187 -2.098495 0.073920
Cs -3.917700 0.892836 -0.841154

Cs2I+.GGG-HI
E=-697.493250
C 2.460472 -1.528688 -0.913629
O 3.262947 -0.614928 -0.740038
N 1.529759 -1.559293 -1.894915
C 0.997710 -0.319946 -2.437034
H 1.779569 0.444460 -2.410033
H 0.699218 -0.469304 -3.483686
C -0.240139 0.046080 -1.589980
O -1.034144 -0.914808 -1.411327
O -0.333732 1.213331 -1.126659
H 0.788568 -2.243275 -1.768380
N -1.755034 -1.322433 2.119537

H -1.025741 -0.738086 2.531058
H -2.285534 -1.685259 2.908877
C -1.067611 -2.432955 1.465231
H -1.570619 -2.715535 0.529376
N 1.066906 -3.007622 0.451279
O 0.838115 -0.954518 1.375679
H -1.011656 -3.335790 2.097140
H 0.646452 -3.912519 0.282419
C 2.423547 -2.743907 0.014980
H 3.083924 -2.522173 0.863039
H 2.803787 -3.633130 -0.503857
Cs 2.084329 1.748712 0.569423
Cs -3.197941 0.549360 -0.139785
C 0.356654 -2.052333 1.095665

Cs2I.GG-HI
E=-490.257103
C 0.836472 -1.118264 -1.553063
C -0.301964 -0.589062 -0.648068
O -0.620344 0.630255 -0.780241
O -0.836203 -1.434080 0.099677
H 1.447474 -0.288977 -1.932295
H 0.380571 -1.609572 -2.423258
N 1.677356 -2.072078 -0.878595
H 1.500066 -3.072090 -0.919374
C 2.464449 -1.676379 0.129335
O 2.647175 -0.489629 0.429088
C 3.117519 -2.800950 0.915582
H 2.589631 -2.829879 1.879847
H 4.150356 -2.481727 1.134377
N 2.984908 -4.089738 0.259464
H 3.745811 -4.234888 -0.400195
H 3.041317 -4.846764 0.934619
Cs 1.716190 2.212078 0.092240
Cs -3.456462 -0.212948 0.180656

Cs3I2.GGG-HI
E=-708.979176
O -0.851325 1.874249 1.501554
C -0.241762 0.994091 2.159518
O -0.467406 -0.244677 2.168327
C 0.889092 1.489922 3.089535
N 2.113056 0.723024 2.942324
C 2.873998 0.888052 1.848674
C 4.146957 0.040088 1.756338
N 4.554671 -0.073984 0.379264
O 2.605278 1.697174 0.962418
C 3.709122 -0.684159 -0.482833
O 2.763067 -1.366167 -0.087102
C 3.967294 -0.503440 -1.963061
N 2.733037 -0.020363 -2.577218
H 2.006060 -0.722577 -2.428289
H 2.857469 0.010647 -3.588308
H 4.320345 -1.475789 -2.352529
H 4.771356 0.225051 -2.132715
H 5.173055 0.636908 0.010671
H 4.949256 0.523791 2.329343
H 1.100725 2.544364 2.881192
H 3.982703 -0.958178 2.182372
H 2.325434 -0.019046 3.595225
H 0.553634 1.396750 4.130632
Cs 0.677153 2.255983 -1.164746
Cs 0.282312 -2.673017 0.713220
I -1.605676 -0.836940 -2.148571
Cs -3.454187 0.576365 0.982898

Cs3I2.GG-HI
E=-501.747507
C -0.431033 -0.860063 1.966600
O 0.530104 -1.615867 1.675424
O -0.471038 0.393028 1.905177
C -1.691292 -1.583785 2.500528
N -2.923605 -0.911392 2.160453
C -3.266390 -0.748694 0.874571
O -2.592140 -1.197290 -0.060560
C -4.556245 0.003310 0.601734
N -4.354329 0.866449 -0.558126
H -5.244017 1.291798 -0.814310
H -4.113860 0.257688 -1.341290
H -4.839010 0.613970 1.470387
H -5.351328 -0.753087 0.468352
H -3.464018 -0.449376 2.879101
H -1.620343 -1.641053 3.594236
H -1.704811 -2.611980 2.116681
Cs -0.112153 -2.587241 -1.126586
Cs -1.429629 2.272126 -0.193931
I 1.673513 0.787372 -1.984302
Cs 2.787620 0.321885 1.716111

Cs3I2.G-HI
E=-294.507856
C -0.781709 -1.388212 2.770526
N -2.221785 -1.617971 2.688622
C -0.357377 -0.090683 2.056212
O -1.279604 0.687119 1.700140
O 0.882511 0.076756 1.909489
Cs 2.760678 -1.573744 0.378883
I 0.361357 -0.021244 -2.251444
Cs 0.426691 2.822597 0.508554
Cs -2.965626 -0.850522 -0.338897
H -2.477380 -2.368169 3.329116
H -2.664019 -0.778564 3.063373
H -0.248195 -2.230703 2.303679
H -0.394390 -1.316717 3.802825

Cs2I+
E=-11.483636
I 0.000000 0.000000 0.000000
Cs 0.000000 0.000000 3.742012
Cs 0.000000 0.000000 -3.742012

Cs3I2+
E=-22.956584
Cs 0.000000 0.000033 0.000054
I -0.000011 0.003662 -3.780838
Cs -0.000022 0.007218 -7.494656

I 0.000011 -0.003648 3.780842
Cs 0.000022 -0.007264 7.494597

G
E=-283.354905
C -0.640357 -0.783884 -0.137125
N -1.761030 0.117872 0.097684
C 0.689355 -0.035557 -0.004036
O 1.749202 -0.598512 0.107089
O 0.545648 1.290188 -0.068575
H -2.577491 -0.143061 -0.447416
H -2.041670 0.103689 1.075573
H -0.679856 -1.155140 -1.170678
H -0.598338 -1.666320 0.517890
H -0.428227 1.418962 -0.120309

GG
E=-490.574634
N 3.574392 0.317640 -0.497960
H 4.423106 0.767173 -0.165904
H 3.686604 -0.681398 -0.329870
C 2.436372 0.758557 0.280982
H 2.619088 0.850000 1.371116
H 2.092911 1.745418 -0.064681
C 1.321720 -0.263003 0.134755
O 1.551278 -1.464888 0.092907
N 0.061286 0.237681 0.112220
H -0.117175 1.234150 0.072463
C -1.070805 -0.637782 0.025412
H -1.133658 -1.317047 0.889757
H -1.021156 -1.287468 -0.862765
C -2.334164 0.180831 -0.043239
O -2.372993 1.389981 -0.050954
O -3.419830 -0.602785 -0.098344
H -4.185840 -0.008155 -0.146276

GGG
-697.802252
C 1.366488 1.754197 -0.470789
N 1.533377 0.368501 -0.862607
C 1.971162 -0.554068 0.053535
O 2.754360 -0.321935 0.953639
C -0.090060 1.997802 -0.098036
O -0.903015 1.391754 -0.984890
O -0.468591 2.624573 0.861453
C 1.404089 -1.963095 -0.179423
N 0.010447 -1.922936 -0.575054
C -0.882538 -1.293388 0.235216
O -0.550798 -0.794632 1.301823
C -2.327689 -1.227100 -0.237288
N -2.885391 0.039560 0.219605
H 1.999084 1.958406 0.398946
H 1.656635 2.433999 -1.286327
H 0.771255 0.045225 -1.446959
H 1.977883 -2.472027 -0.965256
H 1.541495 -2.503560 0.765985
H -0.294608 -2.345915 -1.440930
H -2.380252 -1.282061 -1.333969
H -2.847119 -2.115450 0.166360
H -1.787597 1.207620 -0.555825
H -3.899572 0.044762 0.140640
H -2.650601 0.148947 1.208242