SUPPORTING INFORMATION

From Weak to Strong Interactions Between Halogen and Noble Gas Atoms in Halonium Complexes

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Computational details

Quantum calculations were carried out with the M06-2X DFT functional, with the aid of the def2tzvpp[1-4] basis set within the context of the Gaussian 16 (Rev. C.01) package[5]. It was pointed out earlier that the DFT method is able to predict correctly the electronic structure of similar cations as those selected within current work[6]. Harmonic frequency analysis of normal modes verified that the optimized geometries of additional model complexes represent true minima. The counterpoise approach proposed by Boys and Bernardi removed basis set superposition error (BSSE)[7]. The MEP (molecular electrostatic potential) of the isolated cationic monomers was analyzed via MultiWFN software[8, 9] in order to compute maxima on the 0.001 au isodensity surface. Graphical post-processing of the MEP was performed using the VMD software[10]. Using the AIMAll program[11], the QTAIM analysis of the electron density topology[12, 13] illuminated bond paths and bond critical points with associated quantum chemical parameters. The NBO method (NBO 7 version) was used to analyze[14] interorbital interactions within complexes and processing the Natural Resonance Theory (NRT) results. Decomposition of the interaction energy into its components was succeeded using the ALMO-EDA protocol[15, 16].

Table S1. Selected geometrical parameters of monomers. Distances in Å, angles in degs.

No.	R(X-C1)/R(X-C2)	θ(C1-X-C2)	No.	R(X-N)	No.	R(X-Xe)
1	1.835/1.931	45.5	**4**	1.693	**7**	2.290
2	1.997/2.092	41.5	**5**	1.857	**8**	2.463

3	2.200/2.295	37.2	**6**	2.061	**9**	2.703

Table S2. MEP maxima at σ-hole belonging to the X atoms (X= Cl, Br, I) on the 0.001 au isodensity surface, in kcal/mol.

No.	$V_{s,max}$	No.	$V_{s,max}$	No.	$V_{s,max}$
1	117.3	**4**	114.2	**7**	140.4
2	121.6	**5**	122.4	**8**	152.0
3	130.0	**6**	135.2	**9**	169.2

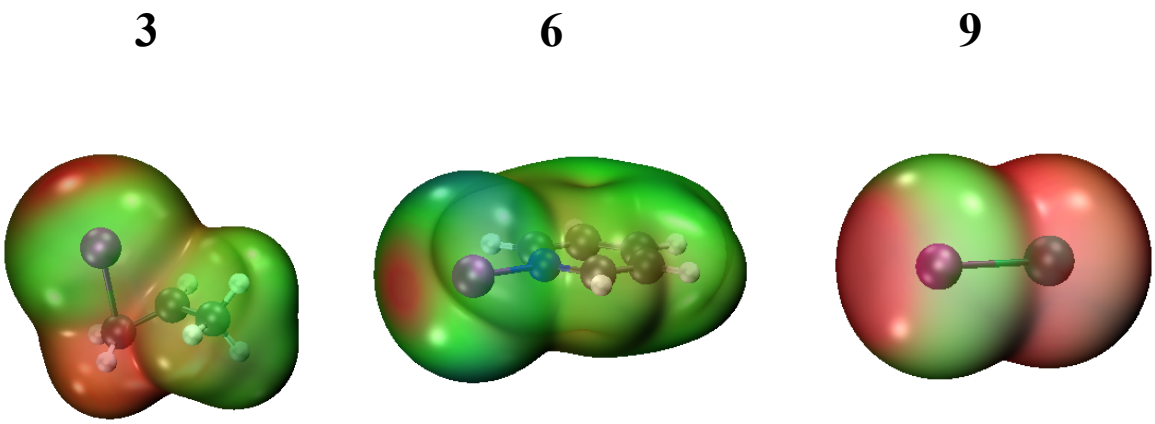

Figure S1. MEP for three selected monomers with the strongest MEP maxima at X atoms within each group of monomers. Color scale from 63 kcal/mol (green) to 125 kcal/mol (red). Color codes: I – purple, Xe – light blue, N – dark blue, C – grey, H – white.

Table S3. Selected angles describing V_{max} location in PrX^+ monomers. Values in degrees.

No.	∠mp-X-V_{max}[a]	∠C1-X-V_{max}	∠C2-X- V_{max}	deviation of the σ-hole location from the C1-C2-X plane, degs
1	22.3	179.0	135.6	0.2
2	9.3	167.9	150.5	2.2
3	5.7	166.7	156.1	0.5

[a] mp refers to midpoint of C1-C2 bond.

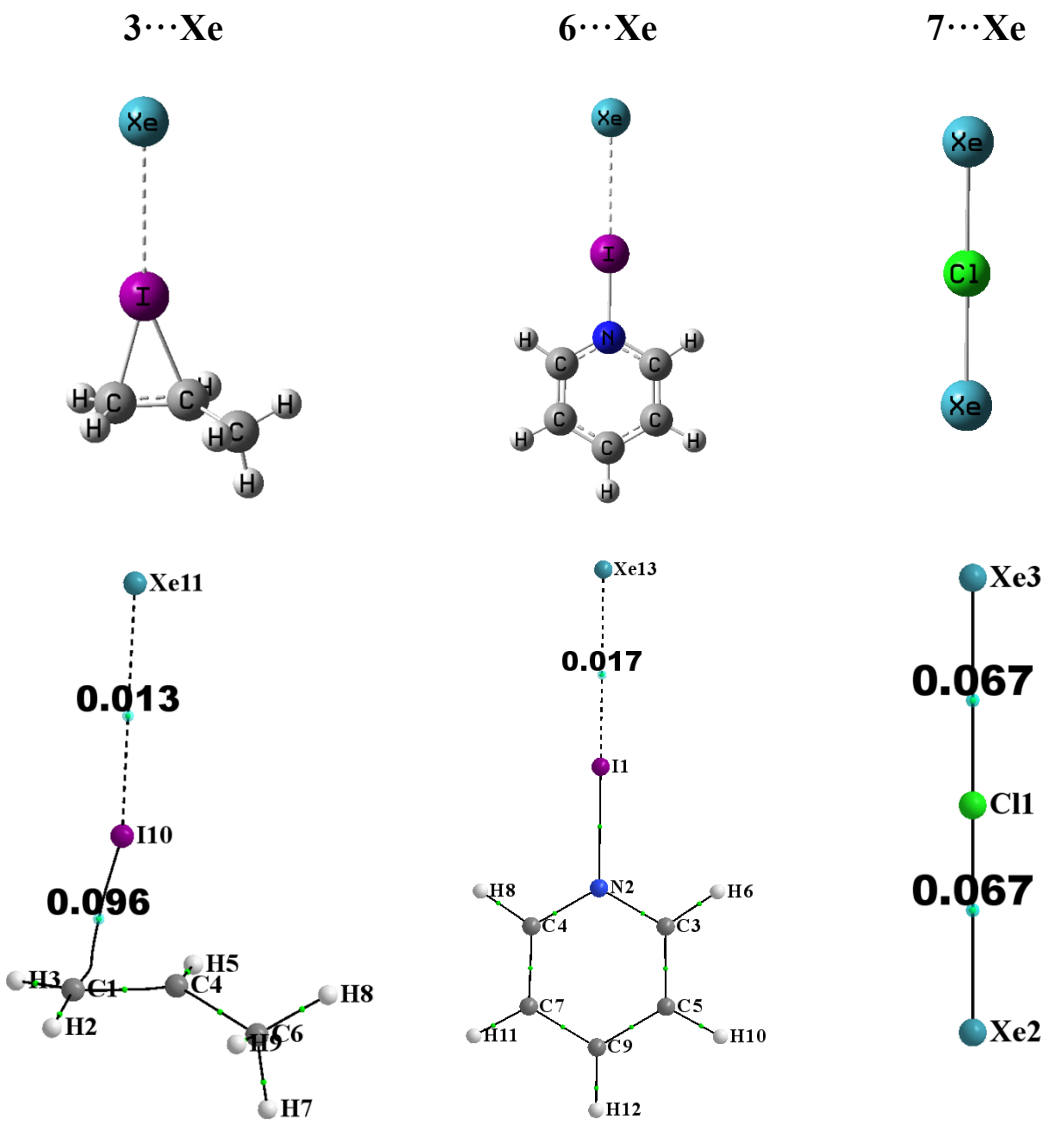

Figure S2. Optimized structures and QTAIM diagrams of strongest dimers in each group. Green points represent BCP. Values of ρ at BCP are given in au.

Table S4. Selected geometrical parameters for the halonium monomers in complexes with single noble gases atoms (Ar, Kr, Xe). Distances in Å, angles in degs.

No.	R(X···Ng)			θ (C-X···Ng or N-X···Ng or Xe-X···Ng)			Δr(C/N/Xe-X) (complex-monomer)		
	Ar	Kr	Xe	Ar	Kr	Xe	Ar	Kr	Xe
1	3.348	3.422	3.548	175.1/139.4[a]	168.5/146.0	162.6/152.1	0.000/0.000[b]	0.002/0.000	0.004/0.002
2	3.365	3.432	3.553	165.2/153.4	166.3/152.4	165.1/153.7	0.002/0.002	0.005/0.004	0.009/0.007
3	3.395	3.464	3.572	165.4/157.6	165.2/157.9	164.9/158.4	0.007/0.006	0.012/0.011	0.020/0.018
4	3.167	3.239	3.364	179.9	179.9	178.6	0.002	0.004	0.008
5	3.153	3.225	3.351	180.0	179.9	179.9	0.005	0.008	0.015

6	3.196	3.274	3.386	180.0	180.0	179.9	0.008	0.014	0.023
7	2.320	2.385	2.569	177.2	178.8	179.4	0.030	0.095	0.279
8	2.502	2.570	2.702	179.2	179.1	179.3	0.039	0.107	0.239
9	2.750	2.801	2.899	178.9	179.2	179.1	0.047	0.098	0.196

[a] C1-X···Ng/ C2-X···Ng. [b] Δr(C1-X)/ Δr(C2-X)

Table S5. Characteristics of complexes; E_{int} – interaction energy, $E^{(2)}$ – second-order interaction energies between LP(Ng) and σ*(X-R) orbitals where X= Cl, Br, I and R= C, N or Xe (both given in kcal/mol), ρ = electron density at bond critical points (QTAIM-derived, in au), ∇^2 = Laplacian of electron density at bond critical points, H = total electron energy density at bond critical points, T1 = values of diagnostic test.

	E_{int} M06-2X			E_{int} CCSD(T)			ρ at BCPs			$E^{(2), a}$		
	Ar	Kr	Xe	Ar	Kr	Xe	Ar	Kr	Xe	Ar	Kr	Xe
1	-0.78	-1.09	-1.58	-0.62	-0.89	-1.22	0.007	0.008	0.009	0.91/0.21	1.22/0.47	1.49/0.93
2	-1.03	-1.50	-2.21	-0.76	-1.17	-1.71	0.008	0.010	0.011	1.10/0.61	1.75/0.93	2.46/1.49
3	-1.48	-2.22	-3.32	-0.85	-1.46	-2.34	0.009	0.011	0.013	1.54/1.01	2.30/1.57	3.41/2.46
4	-1.04	-1.47	-2.14	-0.58	-0.88	-1.28	0.009	0.011	0.012	2.45	3.53	4.72
5	-1.53	-2.26	-3.34	-0.83	-1.43	-2.31	0.012	0.013	0.015	4.37	6.32	8.53
6	-2.33	-3.43	-5.01	-1.09	-2.04	-3.49	0.013	0.015	0.017	6.64	9.31	12.98
7	-3.36	-8.02	-25.56	-1.14	-3.65	-18.01	0.021	0.039	0.067	13.81	43.27	152.45
8	-4.63	-9.98	-23.63	-2.28	-5.80	-17.54	0.024	0.042	0.059	20.23	56.95	129.74
9	-5.90	-10.45	-19.87	-3.25	-7.01	-15.81	0.023	0.034	0.046	23.03	48.36	91.33

[a] refers to donation to σ*(X-C1)/ σ*(X-C2) orbitals

	∇^2 at BCPs			H at BCPs			T1		
	Ar	Kr	Xe	Ar	Kr	Xe	Ar	Kr	Xe
1	0.029	0.031	0.029	0.002	0.002	0.001	0.011	0.010	0.010
2	0.031	0.033	0.031	0.002	0.001	0.001	0.010	0.010	0.010
3	0.034	0.035	0.033	0.002	0.001	0.001	0.011	0.010	0.010
4	0.041	0.042	0.039	0.002	0.002	0.002	0.013	0.012	0.012

5	0.046	0.046	0.042	0.002	0.002	0.001	0.012	0.011	0.011
6	0.048	0.046	0.042	0.002	0.001	0.000	0.012	0.011	0.011
7	0.128	0.102	0.076	-0.023	-0.018	-0.014	0.012	0.010	0.010
8	0.113	0.086	0.064	-0.016	-0.014	-0.011	0.009	0.008	0.008
9	0.107	0.079	0.056	-0.005	-0.008	-0.008	0.008	0.007	0.008

Table S6. Interaction, binding, and deformation energies (kcal/mol)

	E_{int}			E_b			E_{def}		
	Ar	Kr	Xe	Ar	Kr	Xe	Ar	Kr	Xe
1	-0.78	-1.09	-1.58	-0.78	-1.09	-1.57	0.00	0.00	0.01
2	-1.03	-1.50	-2.21	-1.03	-1.49	-2.19	0.00	0.01	0.02
3	-1.48	-2.22	-3.32	-1.47	-2.19	-3.23	0.01	0.03	0.09
4	-1.04	-1.47	-2.14	-1.03	-1.47	-2.12	0.01	0.00	0.02
5	-1.53	-2.26	-3.34	-1.52	-2.24	-3.27	0.01	0.02	0.07
6	-2.33	-3.43	-5.01	-2.32	-3.39	-4.89	0.01	0.04	0.12
7	-3.36	-8.02	-25.56	-3.03	-6.43	-15.72	0.33	1.59	9.84
8	-4.63	-9.98	-23.63	-4.19	-8.38	-17.35	0.44	1.60	6.28
9	-5.90	-10.45	-19.87	-5.65	-9.54	-16.76	0.25	0.91	3.11

Table S7. Quantum chemical characteristics for FX and X^+ in complexes with single noble gases atoms, where X= Cl, Br, I; E_{int} – interaction energy (kcal/mol) and ρ = electron density at bond critical points (QTAIM-derived, au).

	E_{int} M06-2X			E_{int} CCSD(T)			ρ at BCPs		
	Ar	Kr	Xe	Ar	Kr	Xe	Ar	Kr	Xe
FCl	-0.56	-0.78	-1.12	0.05	0.10	0.15	0.008	0.010	0.011
FBr	-0.92	-1.32	-1.86	0.07	-0.13	-0.36	0.011	0.012	0.013
FI	-1.39	-1.89	-2.57	-0.06	-0.36	-0.75	0.010	0.012	0.012
Cl^+	-66.22	-86.21	-110.81	-49.70	-69.40	-96.02	0.136	0.128	0.116
Br^+	-44.16	-60.75	-81.25	-32.26	-48.17	-70.33	0.096	0.097	0.093
I^+	-25.67	-37.20	-52.23	-17.89	-29.05	-45.23	0.057	0.063	0.066

Table S8. ALMO-EDA decomposition of interaction energies (kcal/mol). ELEC= electrostatic term, PAULI = Pauli repulsion, DISP = dispersion, POL = polarization, CT = charge transfer. Percentage contributions are listed as fraction of sum of attractive elements.

	E_{int}	ELEC	%	PAULI	DISP	%	POL	%	CT	%
1···Ar	-0.78	-1.82	50	2.89	-0.82	22	-0.47	13	-0.56	15
2···Ar	-1.03	-2.20	47	3.67	-1.03	22	-0.59	13	-0.88	19
3···Ar	-1.49	-0.79	17	3.09	-1.61	35	-0.83	18	-1.35	29
4···Ar	-1.03	-2.68	50	4.34	-1.16	22	-0.51	10	-1.02	19
5···Ar	-1.53	-3.59	47	6.10	-1.60	21	-0.76	10	-1.69	22
6···Ar	-2.34	-1.33	18	4.90	-2.31	32	-1.19	16	-2.42	33
7···Ar	-3.38	-2.52	20	9.08	-2.80	22	-1.59	13	-5.54	45
8···Ar	-4.62	-3.20	20	11.32	-3.17	20	-2.32	15	-7.26	46
9···Ar	-5.90	-3.41	19	12.03	-3.78	21	-3.27	18	-7.48	42
1···Kr	-1.09	-2.32	46	3.97	-1.03	20	-0.86	17	-0.85	17
2···Kr	-1.50	-2.80	43	5.08	-1.33	20	-1.07	16	-1.38	21
3···Kr	-2.22	-1.36	19	4.83	-2.08	30	-1.50	21	-2.11	30
4···Kr	-1.48	-1.07	21	3.55	-1.49	30	-0.93	19	-1.53	30
5···Kr	-2.26	-1.69	22	5.46	-2.02	26	-1.35	18	-2.67	35
6···Kr	-3.43	-2.21	20	7.40	-2.89	27	-2.07	19	-3.67	34
7···Kr	-8.06	-7.70	23	25.80	-4.79	14	-3.82	11	-17.55	52
8···Kr	-9.98	-9.21	23	29.57	-5.03	13	-5.78	15	-19.53	49
9···Kr	-10.45	-7.72	22	24.81	-5.34	15	-6.97	20	-15.23	43
1···Xe	-1.57	-0.99	19	3.57	-1.50	29	-1.24	24	-1.40	27

2⋯Xe	-2.22	-1.48	20	5.01	-1.99	28	-1.57	22	-2.19	30
3⋯Xe	-3.32	-2.13	20	7.27	-2.81	27	-2.20	21	-3.46	33
4⋯Xe	-2.15	-1.58	21	5.41	-2.26	30	-1.32	17	-2.40	32
5⋯Xe	-3.33	-2.45	22	7.91	-2.81	25	-1.88	17	-4.10	36
6⋯Xe	-5.01	-3.36	21	10.86	-3.80	24	-2.92	18	-5.79	37
7⋯Xe	-25.48	-20.83	22	67.38	-8.20	9	-8.82	9	-55.02	59
8⋯Xe	-23.63	-18.70	23	57.88	-7.43	9	-10.93	13	-44.45	55
9⋯Xe	-19.87	-14.45	22	44.96	-7.54	12	-11.85	18	-30.99	48

Table S9. NRT results. Percentage of covalent and ionic nature of bond/interaction.

	Covalent	ionic		Covalent	ionic		Covalent	ionic
1⋯Ar	-[a]	-	**1⋯Kr**	-	-	**1⋯Xe**	-	-
2⋯Ar	-	-	**2⋯Kr**	-	-	**2⋯Xe**	-	-
3⋯Ar	-	-	**3⋯Kr**	-	-	**3⋯Xe**	7	93
4⋯Ar	-	-	**4⋯Kr**	3	97	**4⋯Xe**	5	95
5⋯Ar	3	97	**5⋯Kr**	5	95	**5⋯Xe**	8	92
6⋯Ar	4	96	**6⋯Kr**	6	94	**6⋯Xe**	10	90
7⋯Ar	43	57	**7⋯Kr**	55	45	**7⋯Xe**	70	30
8⋯Ar	33	67	**8⋯Kr**	45	55	**8⋯Xe**	59	41
9⋯Ar	20	80	**9⋯Kr**	30	70	**9⋯Xe**	44	56

[a] no detection of bond/interaction in NRT analysis.

Table S10. Percentage of covalent and ionic nature of interaction for FX and X^+ in complexes with a single noble gases atom, as derived from NRT

	Covalent	ionic		Covalent	ionic		Covalent	ionic
FCl⋯Ar	1	99	**FCl⋯Kr**	2	98	**FCl⋯Xe**	3	97
FBr⋯Ar	2	98	**FBr⋯Kr**	3	97	**FBr⋯ Xe**	4	96

FI···Ar	2	98	**FI···Kr**	3	97	**FI··· Xe**	5	95
Cl^{+}···Ar	59	41	**Cl^{+}···Kr**	73	27	**Cl^{+}··· Xe**	91	9
Br^{+}···Ar	45	55	**Br^{+}···Kr**	59	41	**Br^{+}··· Xe**	77	23
I^{+}···Ar	29	71	**I^{+}···Kr**	41	59	**I^{+}··· Xe**	57	43

Table S11. Coordinates of monomers and complexes

MONOMERS

1	C	-5.59744700	4.79229600	0.54079600
	H	-5.06064300	3.85623600	0.63340800
	H	-6.62294300	4.74546000	0.19851500
	C	-4.83183700	6.02033300	0.36626600
	H	-5.38330700	6.88451700	0.01206100
	C	-3.35395700	6.04552000	0.28978500
	H	-3.11151800	6.01741500	-0.77875300
	H	-2.95128500	6.97196900	0.69231200
	H	-2.90039500	5.18406900	0.77478900
	Cl	-5.52924600	5.69405700	2.13723900
2	C	-5.58871300	4.79027000	0.51509700
	H	-5.04948500	3.85495500	0.59978100
	H	-6.61125400	4.74522400	0.16407500
	C	-4.83066600	6.01739300	0.36140100
	H	-5.38098600	6.88425200	0.01152200
	C	-3.35213300	6.04508200	0.27841800
	H	-3.11532200	6.01533300	-0.79195300
	H	-2.94568500	6.97198300	0.67541200
	H	-2.89337100	5.18518600	0.76113400
	Br	-5.57496400	5.70219400	2.29153000
3	C	-5.57814100	4.79112000	0.47945400
	H	-5.03948600	3.85497700	0.56122600
	H	-6.59953800	4.74795700	0.12443500
	C	-4.82947100	6.01031600	0.34758300
	H	-5.37730600	6.88174500	0.00354900
	C	-3.34771400	6.04310700	0.26578100
	H	-3.10748200	6.01128600	-0.80369700
	H	-2.94152400	6.97035200	0.66172600
	H	-2.88636300	5.18562600	0.75064900
	I	-5.63555300	5.71538600	2.47571100
4	Cl	-1.17277200	4.89191100	0.80318200
	N	0.52025700	4.88573500	0.80776700
	C	1.16431200	4.88864500	-0.37392400
	C	1.15792100	4.87818300	1.99289800
	C	2.54033300	4.88374700	-0.38766300
	H	0.54675200	4.89478500	-1.25933800
	C	2.53385000	4.87310700	2.01402100
	H	0.53558100	4.87655800	2.87498500
	C	3.23414200	4.87590500	0.81505200
	H	3.05170400	4.88614100	-1.33886300
	H	3.04006000	4.86702000	2.96796400
	H	4.31548000	4.87199000	0.81794900
5	Br	-1.32885900	4.89217600	0.80285400
	N	0.52811100	4.88583200	0.80777200
	C	1.17733700	4.88869500	-0.37100300
	C	1.17096600	4.87824100	1.99000800
	C	2.55372800	4.88370700	-0.38645300
	H	0.56773000	4.89484600	-1.26198200

	C	2.54724700	4.87311700	2.01288100
	H	0.55652600	4.87648500	2.87767900
	C	3.24892000	4.87581900	0.81509400
	H	3.06367500	4.88602400	-1.33848200
	H	3.05199800	4.86700000	2.96766000
	H	4.33024000	4.87178500	0.81800100
6	I	-1.52762500	4.89360100	0.80210500
	N	0.53363300	4.88563900	0.80782800
	C	1.19439400	4.88842100	-0.36517500
	C	1.18805900	4.87801000	1.98435600
	C	2.57111400	4.88358500	-0.38478900
	H	0.59456500	4.89448700	-1.26293200
	C	2.56466000	4.87302600	2.01131800
	H	0.58340700	4.87606700	2.87890600
	C	3.26824000	4.87588500	0.81514200
	H	3.07962200	4.88593900	-1.33760100
	H	3.06803100	4.86696400	2.96684000
	H	4.34952100	4.87210200	0.81803100
7	Cl	-1.80472800	4.89405300	0.80124800
	Xe	-4.09498400	4.90209400	0.79421800
8	Br	-1.71840200	4.89375000	0.80151300
	Xe	-4.18131000	4.90239700	0.79395300
9	i	-1.33743200	4.89241300	0.80268200
	xe	-4.56228000	4.90373400	0.79278400

DIMERS

	Ar			
1	C	-5.56338200	4.71784200	0.31052200
	H	-5.00355100	3.79414500	0.23310600
	H	-6.59005300	4.70728300	-0.03089500
	C	-4.82967300	5.97593400	0.35305400
	H	-5.40385800	6.87506700	0.15801100
	C	-3.35305000	6.05114800	0.27880100
	H	-3.11661900	6.21899100	-0.77810900
	H	-2.96995700	6.90083300	0.83882300
	H	-2.87580000	5.12896000	0.60231500
	Cl	-5.50445900	5.32567700	2.04104900
	Ar	-5.52022600	6.19040400	5.27527100
2	C	-5.53674200	4.74977100	0.35418700
	H	-4.98613600	3.81825300	0.31250300
	H	-6.57320200	4.72927000	0.04448800
	C	-4.79799800	5.99527400	0.30595600
	H	-5.37028300	6.88803300	0.07761300
	C	-3.32427600	6.05243300	0.16632600
	H	-3.13140900	6.14256300	-0.90933800
	H	-2.91011400	6.93559600	0.64628000
	H	-2.83825700	5.15132000	0.53333600
	Br	-5.45522900	5.46055400	2.22079100
	Ar	-5.80698100	5.96321700	5.52980600
3	C	-5.52126600	4.76314400	0.31220300
	H	-4.97631600	3.82745400	0.29046100
	H	-6.55731700	4.74294200	0.00059100
	C	-4.78637700	5.99268200	0.25906600
	H	-5.35129800	6.88734100	0.01814400
	C	-3.30898900	6.04680800	0.12438500
	H	-3.10904700	6.12064900	-0.95114300
	H	-2.89239300	6.93460600	0.59308800
	H	-2.82480400	5.15068600	0.50624900
	I	-5.50278800	5.50600300	2.39089300

	Ar	-5.90003200	5.91396900	5.73801100
4	Cl	-1.19225600	4.89317500	0.80272700
	N	0.50302900	4.88647100	0.80751100
	C	1.14811400	4.88911600	-0.37364100
	C	1.14146500	4.87866900	1.99224600
	C	2.52379900	4.88365800	-0.38749800
	H	0.53024200	4.89548800	-1.25898200
	C	2.51705400	4.87303400	2.01378500
	H	0.51862500	4.87728900	2.87412700
	C	3.21798200	4.87552600	0.81509500
	H	3.03475200	4.88583300	-1.33892500
	H	3.02263500	4.86673800	2.96806300
	H	4.29928200	4.87115100	0.81810700
	Ar	-4.35938400	4.90131200	0.79419900
5	Br	-1.33953300	4.89249800	0.80221800
	N	0.52198600	4.88595900	0.80749800
	C	1.17217000	4.88877000	-0.37032100
	C	1.16546200	4.87832000	1.98897600
	C	2.54859000	4.88369400	-0.38630200
	H	0.56259300	4.89497400	-1.26136300
	C	2.54176700	4.87310000	2.01275700
	H	0.55081200	4.87661900	2.87654800
	C	3.24373700	4.87575900	0.81520600
	H	3.05865600	4.88599100	-1.33823700
	H	3.04638100	4.86695700	2.96757800
	H	4.32502800	4.87165800	0.81826100
	Ar	-4.49231000	4.90316100	0.79399500
6	I	-1.52204700	4.89289200	0.80169100
	N	0.54706500	4.88564700	0.80763800
	C	1.20786700	4.88740200	-0.36417800
	C	1.20126200	4.87913400	1.98314200
	C	2.58502700	4.88252000	-0.38476700
	H	0.60844400	4.89271000	-1.26226500
	C	2.57828800	4.87411000	2.01142400
	H	0.59679400	4.87809200	2.87786700
	C	3.28163800	4.87580000	0.81528800
	H	3.09428400	4.88403100	-1.33711000
	H	3.08217400	4.86891100	2.96660800
	H	4.36292500	4.87189800	0.81830600
	Ar	-4.71838300	4.90431100	0.79316900
7	Cl	-1.49931100	4.89892000	0.84295600
	Xe	-3.81831700	4.89766600	0.77133800
	Ar	1.30545100	4.88050100	0.79270800
8	Br	-1.44487200	4.89098300	0.78994700
	Xe	-3.94677100	4.90252700	0.80122300
	Ar	1.37946600	4.88357600	0.81583200
9	I	-1.39288400	4.89516300	0.82005600
	Xe	-4.14245800	4.90088000	0.78459900
	Ar	1.52316500	4.88104300	0.80234700
	Kr			
1	C	-5.55735300	4.73229800	0.34002100
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	H	-6.58728900	4.71181300	0.00916700
	C	-4.81954700	5.98772800	0.32676900
	H	-5.39225600	6.88071700	0.10157900
	C	-3.34325300	6.05435500	0.23685000
	H	-3.11496800	6.17617500	-0.82809200
	H	-2.95245000	6.92529900	0.75740800
	H	-2.86658900	5.14480500	0.59517500
	Cl	-5.48077300	5.40741700	2.04626800
	Kr	-5.61471400	6.06151500	5.40221500
2	C	-5.53934000	4.74950500	0.33498400
	H	-4.98948500	3.81753400	0.29479500
	H	-6.57340300	4.73120400	0.01739600

	C	-4.79979000	5.99361900	0.29831600
	H	-5.36901400	6.88811900	0.06929300
	C	-3.32462300	6.05056800	0.17294400
	H	-3.12082700	6.14610700	-0.90013900
	H	-2.91455000	6.93081500	0.66171400
	H	-2.84287500	5.14729300	0.54026300
	Br	-5.47319400	5.45256300	2.20778700
	Kr	-5.78352500	5.97895700	5.58459500
3	C	-5.52089100	4.76499700	0.30383900
	H	-4.97698800	3.82871800	0.28289500
	H	-6.55792100	4.74519600	-0.00433900
	C	-4.78647900	5.99260200	0.25027200
	H	-5.35083900	6.88812900	0.01137900
	C	-3.30882400	6.04684100	0.11691900
	H	-3.10707600	6.12255900	-0.95804300
	H	-2.89251000	6.93347700	0.58805700
	H	-2.82539600	5.14991700	0.49788500
	I	-5.50089800	5.50703000	2.38788300
	Kr	-5.90280300	5.90681700	5.80520200
4	Cl	-1.18865000	4.89368400	0.80216200
	N	0.50876800	4.88679600	0.80718000
	C	1.15408600	4.88906900	-0.37356500
	C	1.14706200	4.87911900	1.99171100
	C	2.52985900	4.88332700	-0.38746700
	H	0.53636000	4.89536700	-1.25901100
	C	2.52272600	4.87320700	2.01373700
	H	0.52407500	4.87803300	2.87349300
	C	3.22385800	4.87529700	0.81519700
	H	3.04100900	4.88518800	-1.33877400
	H	3.02819300	4.86699900	2.96806000
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	Kr	-4.42715400	4.90069900	0.79570400
5	Br	-1.33745100	4.89189000	0.80318400
	N	0.52805800	4.88551300	0.80803700
	C	1.17793900	4.88847000	-0.36949200
	C	1.17188100	4.87803100	1.98887100
	C	2.55450000	4.88374100	-0.38628100
	H	0.56818800	4.89453300	-1.26044000
	C	2.54833900	4.87315400	2.01270300
	H	0.55755100	4.87619000	2.87668800
	C	3.24997500	4.87601000	0.81499900
	H	3.06438200	4.88616600	-1.33829300
	H	3.05330700	4.86714700	2.96731800
	H	4.33126000	4.87221300	0.81776100
	Kr	-4.56259000	4.90440100	0.79175800
6	I	-1.52115900	4.89293600	0.80213400
	N	0.55362300	4.88554700	0.80788300
	C	1.21455300	4.88711800	-0.36339800
	C	1.20822100	4.87925200	1.98270100
	C	2.59183100	4.88228200	-0.38466900
	H	0.61502500	4.89227100	-1.26147300
	C	2.58537000	4.87427600	2.01135400
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	C	3.28864900	4.87579000	0.81522400
	H	3.10100300	4.88366000	-1.33704200
	H	3.08939200	4.86926900	2.96645400
	H	4.36991900	4.87195100	0.81811900
	Kr	-4.79494400	4.90475400	0.79197300
7	Cl	-1.43671800	4.89524500	0.81942500
	Xe	-3.82236000	4.89968600	0.78509900
	Kr	1.24690200	4.88215600	0.80247900
8	Br	-1.38878600	4.89449400	0.81557600
	Xe	-3.95906900	4.90061100	0.78773500
	Kr	1.33567800	4.88198100	0.80369200

9	I	-1.36590100	4.89430200	0.81487500
	Xe	-4.16693100	4.90140500	0.78753900
	Kr	1.52065600	4.88137900	0.80458800
	Xe			
1	C	-5.55135900	4.75044400	0.36505800
	H	-5.00434300	3.81637100	0.33893000
	H	-6.58686300	4.72955300	0.05227100
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	H	-5.37389500	6.88846900	0.06199900
	C	-3.32914300	6.05067100	0.18959700
	H	-3.11593800	6.13941000	-0.88164700
	H	-2.92404800	6.93329100	0.67858200
	H	-2.85370800	5.14838500	0.56738300
	Cl	-5.44205400	5.47391500	2.05199700
	Xe	-5.74481100	5.95792900	5.55377100
2	C	-5.53687900	4.75298300	0.32849800
	H	-4.98850400	3.81999500	0.29306300
	H	-6.57240800	4.73378100	0.01597200
	C	-4.79720400	5.99491800	0.28330100
	H	-5.36580700	6.88915700	0.05192400
	C	-3.32201200	6.05000500	0.15542200
	H	-3.11884600	6.14060000	-0.91813200
	H	-2.91037600	6.93167700	0.64027000
	H	-2.84093800	5.14781000	0.52629700
	Br	-5.46559400	5.46620400	2.20193700
	Xe	-5.81205800	5.95915400	5.70339700
3	C	-5.51810400	4.76600800	0.29245300
	H	-4.97459100	3.82957200	0.27089300
	H	-6.55753000	4.74563200	-0.00723500
	C	-4.78628900	5.99174400	0.23711900
	H	-5.35181300	6.88802500	0.00399800
	C	-3.30878500	6.04861500	0.10230100
	H	-3.10711900	6.12963300	-0.97218400
	H	-2.89308200	6.93334500	0.57756300
	H	-2.82410400	5.15053600	0.47893900
	I	-5.49211800	5.50503500	2.38630600
	Xe	-5.91709200	5.89813800	5.91179300
4	Cl	-1.18213700	4.87712500	0.81776800
	N	0.51892100	4.87668200	0.81639400
	C	1.15871100	4.88147400	-0.36692200
	C	1.16247400	4.87381300	1.99761800
	C	2.53448700	4.88400800	-0.38756000
	H	0.53681600	4.88338900	-1.24948600
	C	2.53839000	4.87621300	2.01361300
	H	0.54358000	4.87004200	2.88228400
	C	3.23399000	4.88163900	0.81189500
	H	3.04122400	4.88812200	-1.34120100
	H	3.04840500	4.87411000	2.96550700
	H	4.31528600	4.88409000	0.81010600
	Xe	-4.54480700	4.92675100	0.75679700
5	Br	-1.33314800	4.89181100	0.80310000
	N	0.53875700	4.88543700	0.80802600
	C	1.18850700	4.88838600	-0.36889800
	C	1.18240200	4.87798600	1.98827700
	C	2.56525800	4.88369600	-0.38621300
	H	0.57879100	4.89441600	-1.25990600
	C	2.55904800	4.87314600	2.01268400
	H	0.56807400	4.87613400	2.87613200
	C	3.26067300	4.87600200	0.81503700
	H	3.07525900	4.88612200	-1.33814000
	H	3.06409600	4.86716800	2.96723500
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	Xe	-4.68432200	4.90490900	0.79166400

6	I	-1.52067400	4.89264500	0.80234500
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	C	1.21824600	4.87826900	1.98192500
	C	2.60194200	4.88313500	-0.38461500
	H	0.62477000	4.89359700	-1.26055600
	C	2.59563400	4.87339600	2.01125800
	H	0.61387600	4.87667500	2.87685900
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	H	3.11118700	4.88525600	-1.33692400
	H	3.09985500	4.86774800	2.96622500
	H	4.38010000	4.87210100	0.81797700
	Xe	-4.90637000	4.90561100	0.79165300
7	Cl	-1.33737700	4.89102500	0.79315700
	Xe	-3.90624800	4.90210900	0.79945400
	Xe	1.23144900	4.88395200	0.81439100
8	Br	-1.33742700	4.89392000	0.81303000
	Xe	-4.03973000	4.90113400	0.78912900
	Xe	1.36498000	4.88203300	0.80484400
9	I	-1.33735400	4.89019400	0.78745300
	Xe	-4.23675700	4.90369300	0.80134500
	Xe	1.56193400	4.88319900	0.81820400

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