Table 1. Bromine GTO Basis set

Function	Exponent	Prefactor
s	9659.390000	0.000371
	1455.960000	0.002571
	325.914000	0.008485
	46.565700	0.078222
	18.246900	-0.397149
	3.802010	0.685864
	1.786320	0.486819
	0.602714	0.034913
	0.284014	-0.006573
	0.120271	0.001642
s	9659.390000	-0.000152
	1455.960000	-0.001008
	325.914000	-0.003609
	46.565700	-0.027872
	18.246900	0.151317
	3.802010	-0.351497
	1.786320	-0.410703
	0.602714	0.347316
	0.284014	0.675491
	0.120271	0.244008
s	0.602714	1.000000
s	0.284014	1.000000
s	0.120271	1.000000
p	492.187000	0.000472
	92.364200	0.005494
	27.071800	-0.088030
	7.265390	0.343485
	3.484810	0.510208
	1.640480	0.248631
	0.648570	0.022201
	0.256407	-0.000419
	0.095304	0.000656
p	492.187000	-0.000158
	92.364200	-0.001344
	27.071800	0.024616
	7.265390	-0.112532
	3.484810	-0.179775
	1.640480	-0.073661
	0.648570	0.348734
	0.256407	0.557948
	0.095304	0.266456
p	0.766600	1.000000
p	0.118200	1.000000
d	338.996000	0.001524
	103.217000	0.015673
	42.363800	0.072400
	18.435600	0.186303
	8.372540	0.323881
	3.802220	0.374534
d	1.686770	1.000000
d	0.677520	1.000000
d	0.255300	1

Table 2. Iodine GTO Basis set

Function	Exponent	Prefactor
s	5546.500000	0.000156
	838.214000	0.000986
	182.187000	0.002792
	31.212300	-0.043251
	19.531400	0.234134
	8.240990	-0.750943
	2.194550	0.882968
	1.109110	0.462061
	0.374641	0.022286
	0.081061	0.001102
s	5546.500000	-0.000073
	838.214000	-0.000508
	182.187000	-0.001158
	31.212300	0.012193
	19.531400	-0.087854
	8.240990	0.338200
	2.194550	-0.576550
	1.109110	-0.409298
	0.374641	0.567459
	0.081061	0.143231
s	0.374641	1.000000
s	0.177080	1.000000
s	0.100100	1.000000
p	188.988000	0.000585
	21.286800	0.036923
	10.039600	-0.235324
	3.451800	0.341483
	1.974560	0.534788
	1.024200	0.265141
	0.449437	0.025787
	0.186648	0.000522
	0.073481	0.000606
p	188.988000	-0.000256
	21.286800	-0.011682
	10.039600	0.083192
	3.451800	-0.156970
	1.974560	-0.224518
	1.024200	-0.114451
	0.449437	0.375356
	0.186648	0.575136
	0.073481	0.245917
p	0.598100	1.000000
p	0.096180	1.000000
d	132.662000	0.000572
	37.605400	0.004402
	10.389100	-0.040922
	6.490170	0.099661
	3.454510	0.322663
	1.844130	0.400343
d	0.962478	1.000000
d	0.472853	1.000000
d	0.193200	1.000000

Table 3. Lattice parameters

	a_0 (Angstrom)
LiF	4.01
LiCl	5.11
LiBr	5.46
LiI	5.97
NaF	4.61
NaCl	5.60
NaBr	5.93
NaI	6.42
KF	5.31
KCl	6.25
KBr	6.56
KI	7.04

Table 4. MPD All Electrons results. V is the volume of primitive unit cell (V_cell) in bohr^3. The data for cationic (M^+) and anionic (X^-) domains are given: p is the probability; V% is the volume of the domain in percentage of V; μ is the average number of electrons in the domain.

	V	$p(M^+)$	$V\%(M^+)$	$\mu(M^+)$	$p(X^-)$	$V\%(X^-)$	$\mu(X^-)$
LiF	108.79	0.93	12.68	2.05	0.72	86.42	9.94
LiCl	224.58	0.94	7.02	2.04	0.65	91.75	17.92
LiBr	274.61	0.95	6.00	2.03	0.60	91.23	25.91
LiI	359.69	0.95	4.95	2.03	0.57	96.30	25.93
NaF	165.18	0.87	27.12	10.05	0.79	69.89	9.95
NaCl	295.49	0.89	15.06	10.06	0.71	81.08	17.96
NaBr	350.92	0.89	13.12	10.05	0.67	82.86	25.90
NaI	447.04	0.90	10.67	10.04	0.63	89.38	25.94
KF	252.74	0.82	49.23	18.09	0.78	47.59	10.00
KCl	418.64	0.82	28.12	18.10	0.77	68.20	18.01
KBr	476.26	0.82	25.10	18.10	0.74	71.33	25.99
KI	589.15	0.82	21.55	18.10	0.71	76.64	25.98

Table 5. ELF All Electrons results. V is the volume of primitive unit cell (V_cell) in bohr^3. The data for cationic (M^+) and anionic (X^-) domains are given: p is the probability; V% is the volume of the domain in percentage of V; μ is the average number of electrons in the domain.

	V	$p(M^+)$	$V\%(M^+)$	$\mu(M^+)$	$p(X^-)$	$V\%(X^-)$	$\mu(X^-)$
LiF	108.79	0.93	13.01	2.06	0.67	87.07	9.88
LiCl	224.58	0.94	7.42	2.04	0.64	92.35	17.93
LiBr	274.61	0.95	6.31	2.04	0.60	94.07	25.92
LiI	359.69	0.95	5.00	2.03	0.57	96.25	25.88
NaF	165.18	0.87	27.36	10.07	0.78	72.15	9.96
NaCl	295.49	0.89	16.14	10.08	0.71	85.00	17.98
NaBr	350.92	0.89	13.67	10.07	0.67	85.52	25.92
NaI	447.04	0.90	11.41	10.07	0.63	88.51	25.92
KF	252.74	0.82	51.18	18.11	0.77	48.76	10.00
KCl	418.64	0.81	31.34	18.14	0.77	69.09	18.00
KBr	476.26	0.82	27.41	18.14	0.74	72.30	25.99
KI	589.15	0.82	21.92	18.12	0.71	77.31	26.00

Table 6. QTAIM All Electrons Results. V is the volume of primitive unit cell (V_cell) in bohr^3. The data for cationic (M^+) and anionic (X^-) domains are given: p is the probability; V% is the volume of the domain in percentage of V; μ is the average number of electrons in the domain.

	V	p(M^+)	V%(M^+)	μ(M^+)	p(X^-)	V%(X^-)	μ(X^-)
LiF	108.79	0.91	17.75	2.11	0.71	82.01	9.89
LiCl	224.58	0.92	11.16	2.11	0.64	88.51	17.87
LiBr	274.61	0.93	9.83	2.10	0.59	90.34	25.86
LiI	359.69	0.94	8.02	2.08	0.56	92.71	25.83
NaF	165.18	0.85	35.91	10.15	0.77	64.49	9.89
NaCl	295.49	0.86	21.57	10.16	0.70	78.97	17.90
NaBr	350.92	0.87	18.57	10.14	0.66	80.95	25.85
NaI	447.04	0.87	15.87	10.13	0.62	83.89	25.84
KF	252.74	0.82	54.62	18.11	0.78	45.53	9.98
KCl	418.64	0.78	39.86	18.26	0.75	60.93	17.89
KBr	476.26	0.78	34.64	18.25	0.72	65.01	25.88
KI	589.15	0.78	28.33	18.25	0.69	70.85	25.86

Table 7. MPD ECP results. V is the volume of primitive unit cell (V_cell) in bohr^3. The data for anionic (X^-) domains are given: p is the probability; V% is the volume of the domain in percentage of V; μ is the average number of electrons in the domain.

	V	p(X^-)	V%(X^-)	μ(X^-)
LiF	108.79	0.75	96.24	9.95
LiCl	224.58	0.66	98.08	17.96
LiBr	274.61	0.61	98.01	25.95
LiI	359.69	0.59	100.79	25.95
NaF	165.18	0.89	94.00	10.01
NaCl	295.49	0.78	94.24	18.01
NaBr	350.92	0.73	96.12	25.98
NaI	447.04	0.68	97.62	25.95
KF	252.74	0.99	98.22	10.04
KCl	418.64	0.94	94.03	18.07
KBr	476.26	0.91	93.54	26.04
KI	589.15	0.83	101.89	26.09

Table 8 ELF ECP results. V is the volume of primitive unit cell (V_cell) in bohr^3. The data for anionic (X^-) domains are given: p is the probability; V% is the volume of the domain in percentage of V; μ is the average number of electrons in the domain.

	V	p(X^-)	V%(X^-)	μ(X^-)
LiF	108.79	0.75	99.87	9.96
LiCl	224.58	0.66	100.26	17.97
LiBr	274.61	0.61	100.27	25.95
LiI	359.69	0.58	99.94	25.89
NaF	165.18	0.89	100.04	10.02
NaCl	295.49	0.78	99.91	18.04
NaBr	350.92	0.73	99.37	25.98
NaI	447.04	0.68	99.56	25.96
KF	252.74	0.99	99.79	10.03
KCl	418.64	0.94	99.43	18.08
KBr	476.26	0.91	99.71	26.06
KI	589.15	0.84	100.66	26.10

Table 9. QTAIM ECP results. V is the volume of primitive unit cell (V_cell) in bohr^3. The data for anionic (X^-) domains are given: p is the probability; V% is the volume of the domain in percentage of V; μ is the average number of electrons in the domain.

	V	$p(X^-)$	$V\%(X^-)$	$\mu(X^-)$
LiF	108.79	0.75	99.87	9.96
LiCl	224.58	0.66	100.26	17.97
LiBr	274.61	0.61	100.26	25.95
LiI	359.69	0.58	99.94	25.89
NaF	165.18	0.89	100.03	10.02
NaCl	295.49	0.78	99.90	18.04
NaBr	350.92	0.73	99.36	25.98
NaI	447.04	0.68	99.55	25.96
KF	252.74	0.99	99.84	10.03
KCl	418.64	0.94	99.46	18.08
KBr	476.26	0.91	100.03	26.08
KI	589.15	0.84	100.67	26.10