Supporting Information

Theoretical investigation of energetic salts with pentazolate anion

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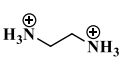
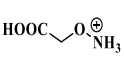
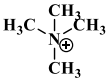
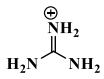
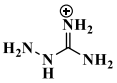
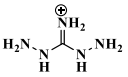
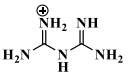
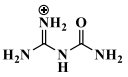
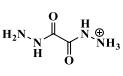
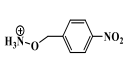
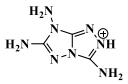
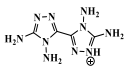
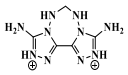
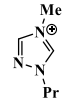
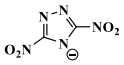
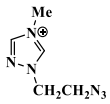
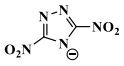
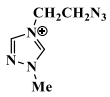
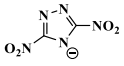
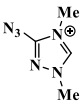
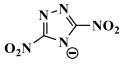
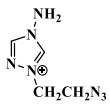
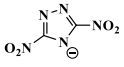
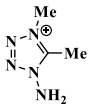
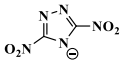
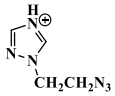
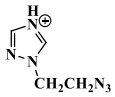
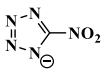
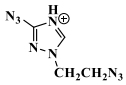
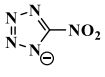
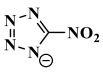
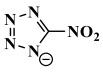
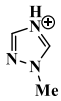
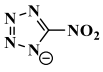
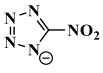
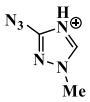
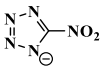
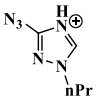
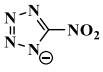
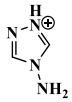
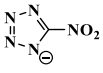
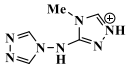
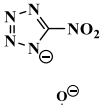
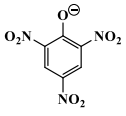
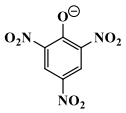
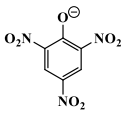
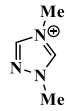
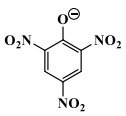
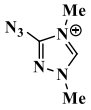
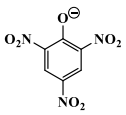
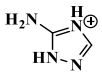
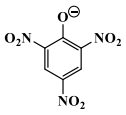
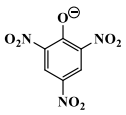
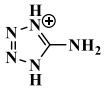
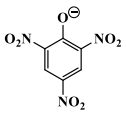
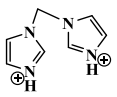
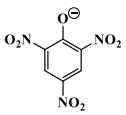
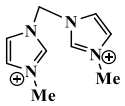
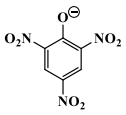
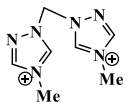
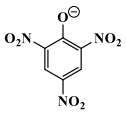
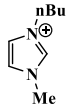
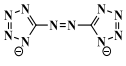
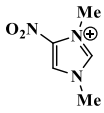
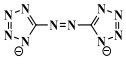
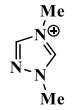
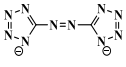
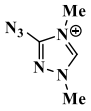
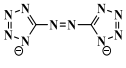
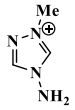
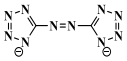
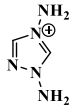
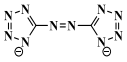
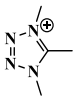
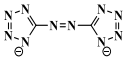
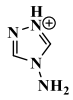
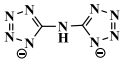
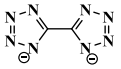
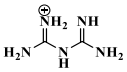
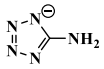
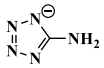
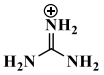
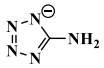
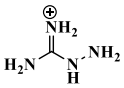
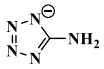
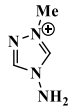
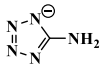
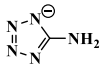
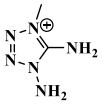
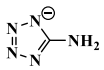
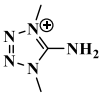
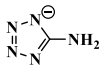
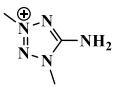
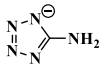
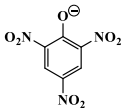
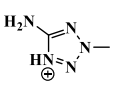
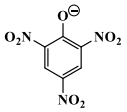
Table S1 Ionization potential of cations and electron affinity of anions

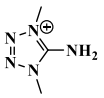
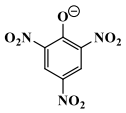
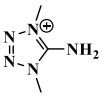
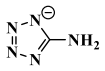
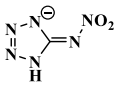
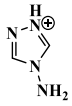
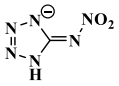
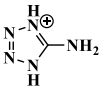
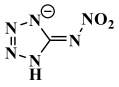
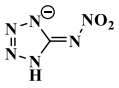
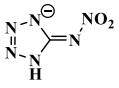
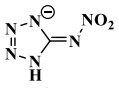
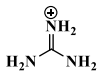
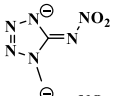
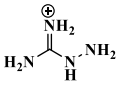
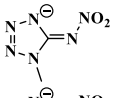
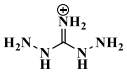
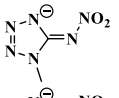
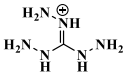
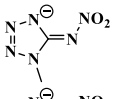
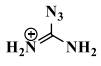
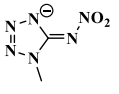
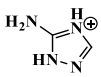
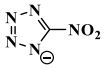
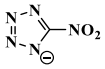
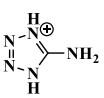
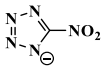
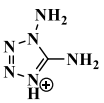
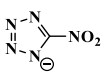
salts	cation	EA(cation)		anion	IP(anion)	
		B3LYP/6-311++G(d,p)	B3LYP/aug-cc-pVTZ		B3LYP/6-311++G(d,p)	B3LYP/aug-cc-pVTZ
1		4.74	4.74		5.72	5.60
2		4.39	4.38		5.72	5.60
3		4.71	4.68		5.72	5.60
4		8.00	7.98		5.72	5.60
5		4.73	4.66		5.72	5.60
6		3.13	3.14		5.72	5.60
7		3.61	3.63		5.72	5.60
8		3.49	3.49		5.72	5.60
9		3.44	3.43		5.72	5.60
10		3.39	3.39		5.72	5.60
11		3.55	3.54		5.72	5.60
12		4.15	4.12		5.72	5.60

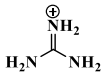
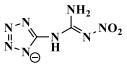
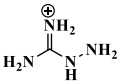
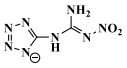
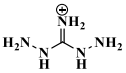
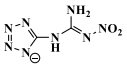
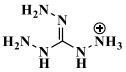
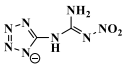
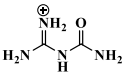
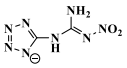
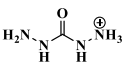
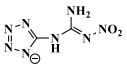
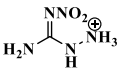
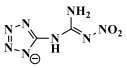
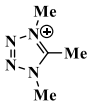
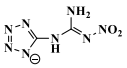
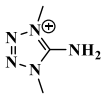
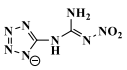
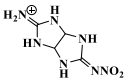
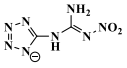
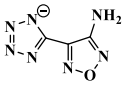
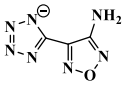
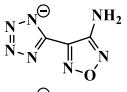
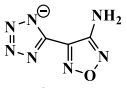
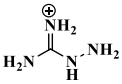
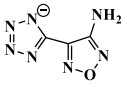
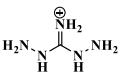
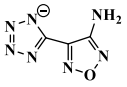
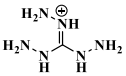
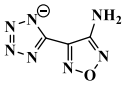
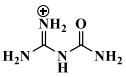
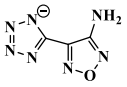
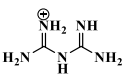
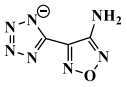
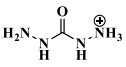
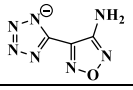
13		4.55	4.52		5.72	5.60
14		3.52	3.52		5.72	5.60
15		2.98	2.99		5.72	5.60
16		3.25	3.23		5.72	5.60
17		7.60	7.60		5.72	5.60
18		3.71	3.70		6.11	5.98
19		4.00	3.98		6.11	5.98
20		3.97	3.94		6.11	5.98
21		4.14	4.09		6.11	5.98
22		3.85	3.83		6.11	5.98
23		3.85	3.83		6.11	5.98
24		4.12	1.86		4.98	4.88
25		4.12	1.86		5.99	5.86
26		4.37	4.29		5.99	5.86
27		4.33	4.26		4.98	4.88
28		4.28	4.25		4.98	4.88

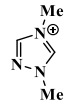
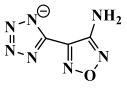
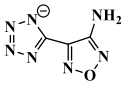
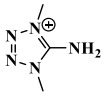
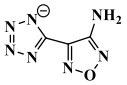
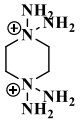
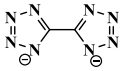
29		4.00	3.97		4.98	4.88
30		4.55	4.47		4.98	4.88
31		4.28	4.22		4.98	4.88
32		3.94	3.92		4.98	4.88
33		3.32	3.33		4.98	4.88
34		3.83	4.14		5.05	4.96
35		4.33	4.26		5.99	5.86
36		4.28	4.25		5.99	5.86
37		4.00	3.97		5.99	5.86
38		4.55	4.47		5.99	5.86
39		4.28	4.22		5.99	5.86
40		4.11	4.04		5.99	5.86
41		3.94	3.92		5.99	5.86
42		4.18	4.14		5.99	5.86
43		4.55	4.47		5.23	5.12

44		4.28	4.25		5.23	5.12
45		4.00	3.97		5.23	5.12
46		3.88	3.87		5.23	5.12
47		4.14	4.09		5.23	5.12
48		3.61	3.61		5.23	5.12
49		3.94	3.92		5.23	5.12
50		3.99	3.97		5.23	5.12
51		7.54	7.59		5.23	5.12
52		7.10	7.11		5.23	5.12
53		7.56	7.52		5.23	5.12
54		3.38	3.38		12.75	1.05
55		5.02	4.98		12.75	1.05
56		3.88	3.87		12.75	1.05
57		4.14	4.09		12.75	1.05

58		3.72	3.71		12.75	1.05
59		4.04	4.01		12.75	1.05
60		3.93	3.88		12.75	1.05
61		3.94	3.92		-0.19	-0.27
62		3.94	3.92		0.33	0.23
63		3.39	3.39		3.48	3.41
64		3.94	3.92		3.48	3.41
65		3.61	3.63		3.48	3.41
66		3.49	3.49		3.48	3.41
67		3.72	3.71		3.48	3.41
68		3.59	3.58		3.48	3.41
69		3.61	3.61		3.48	3.41
70		3.57	3.56		3.48	3.41
71		4.24	4.20		3.48	3.41
72		3.79	3.78		5.23	5.12
73		4.45	4.41		5.23	5.12

74		3.57	3.56		5.23	5.12
75		3.57	3.56		3.48	3.41
76		3.79	3.78		4.55	4.46
77		3.94	3.92		4.55	4.46
78		3.99	3.97		4.55	4.46
79		4.28	4.25		4.55	4.46
80		3.81	3.78		4.55	4.46
81		4.55	4.47		4.55	4.46
82		3.61	3.63		4.40	4.33
83		3.49	3.49		4.40	4.33
84		3.38	3.38		4.40	4.33
85		3.32	3.32		4.40	4.33
86		4.64	4.57		4.40	4.33
87		3.61	3.61		5.99	5.86
88		4.12	4.08		5.99	5.86
89		3.99	3.97		5.99	5.86
90		3.86	3.80		5.99	5.86

91		3.61	3.63		4.74	4.66
92		3.49	3.49		4.74	4.66
93		3.38	3.38		4.74	4.66
94		3.19	3.21		4.74	4.66
95		3.55	3.54		4.74	4.66
96		3.74	3.72		4.74	4.66
97		4.26	4.22		4.74	4.66
98		3.93	3.88		4.74	4.66
99		3.57	3.56		4.74	4.66
100		3.80	3.76		4.74	4.66
101		4.74	4.74		4.87	4.76
102		3.60	3.60		4.87	4.76
103		4.39	4.38		4.87	4.76
104		3.61	3.63		4.87	4.76
105		3.49	3.49		4.87	4.76
106		3.38	3.38		4.87	4.76
107		3.32	3.32		4.87	4.76
108		3.55	3.54		4.87	4.76
109		3.39	3.39		4.87	4.76
110		3.74	3.72		4.87	4.76

111		3.88	3.87		4.87	4.76
112		3.93	3.88		4.87	4.76
113		3.57	3.56		4.87	4.76
114		6.98	6.95		0.33	0.23
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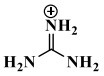
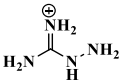
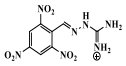
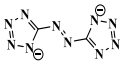
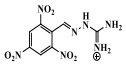
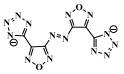
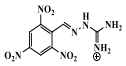
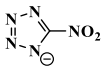
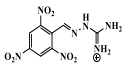
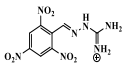
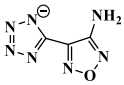
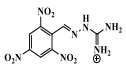
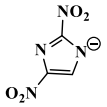
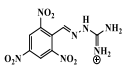
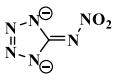
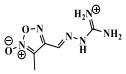
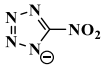
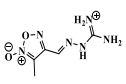
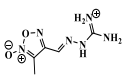
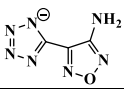
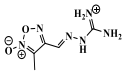
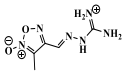
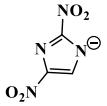
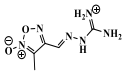
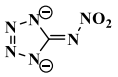
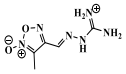
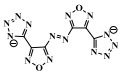
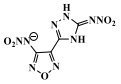
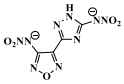
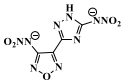
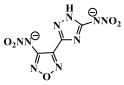
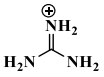
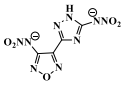
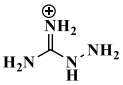
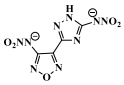
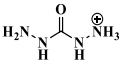
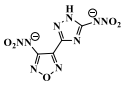
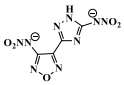
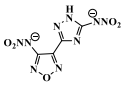
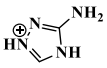
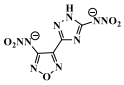
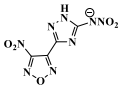
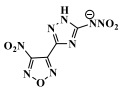
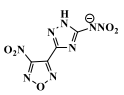
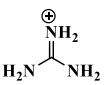
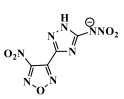
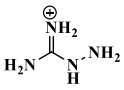
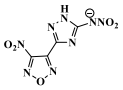
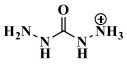
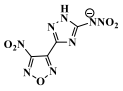
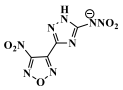
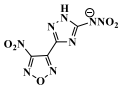
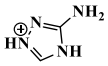
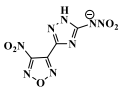
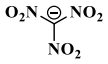
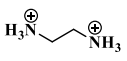
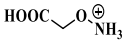
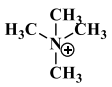
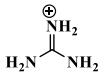
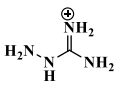
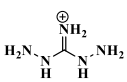
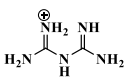
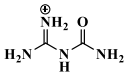
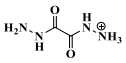
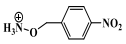
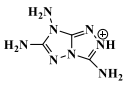
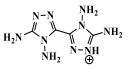
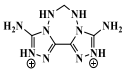
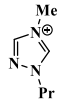
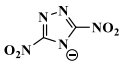
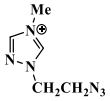
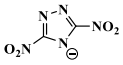
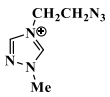
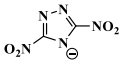
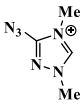
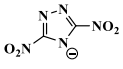
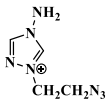
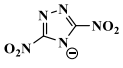
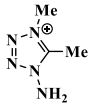
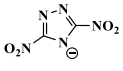
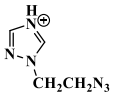
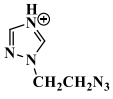
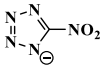
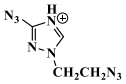
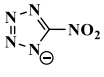
117		3.61	3.63		4.54	4.44
118		3.49	3.49		4.54	4.44
119		5.34	5.24		1.14	1.05
120		5.34	5.24		3.03	2.57
121		5.34	5.24		5.99	5.86
122		5.34	5.24		4.52	4.44
123		5.34	5.24		4.87	4.76
124		5.34	5.24		5.29	5.18
125		5.34	5.24		-0.53	-0.60
126		4.49	4.48		5.99	5.86
127		4.49	4.48		4.52	4.44
128		4.49	4.48		4.87	4.76

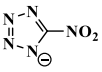
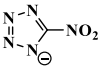
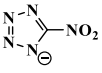
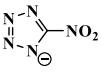
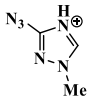
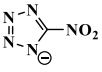
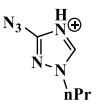
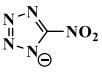
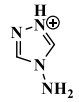
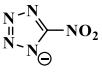
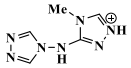
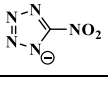
129		4.49	4.48		4.54	4.44
130		4.49	4.48		5.29	5.18
131		4.49	4.48		-0.53	-0.60
132		4.49	4.48		3.03	2.57
133		4.28	4.25		5.06	4.98
134		4.74	4.74		1.63	1.53
135		4.39	4.38		1.63	1.53
136		4.71	4.68		1.63	1.53
137		3.61	3.63		1.63	1.53
138		3.49	3.49		1.63	1.53
139		3.74	3.72		1.63	1.53
140		4.28	4.25		1.63	1.53
141		3.59	3.92		1.63	1.53
142		3.80	3.78		1.63	1.53
143		4.74	4.74		4.86	4.77
144		4.39	4.38		4.86	4.77
145		4.71	4.68		4.86	4.77
146		3.61	3.63		4.86	4.77

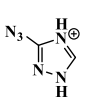
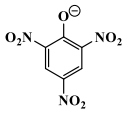
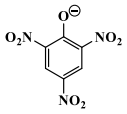
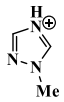
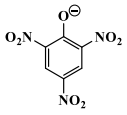
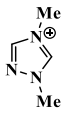
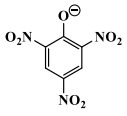
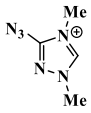
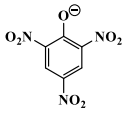
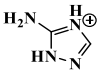
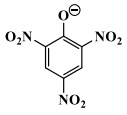
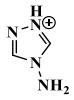
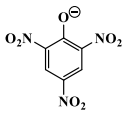
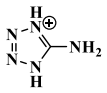
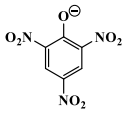
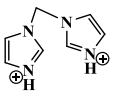
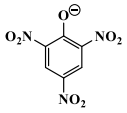
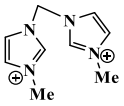
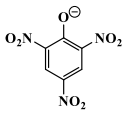
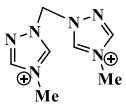
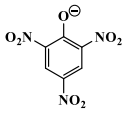
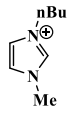
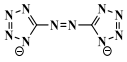
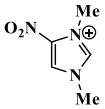
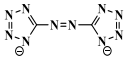
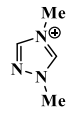
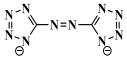
147		3.49	3.49		4.86	4.77
148		3.74	3.72		4.86	4.77
149		4.28	4.25		4.86	4.77
150		3.59	3.92		4.86	4.77
151		3.80	3.78		4.86	4.77
152		4.39	4.38		5.25	5.13

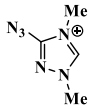
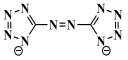
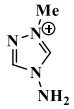
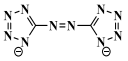
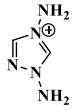
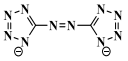
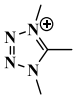
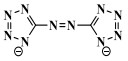
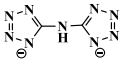
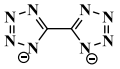
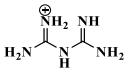
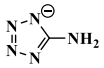
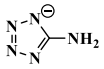
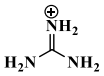
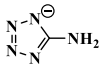
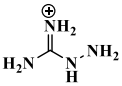
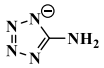
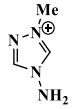
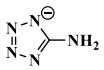
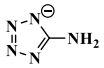
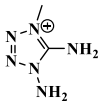
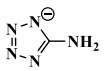
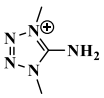
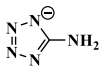
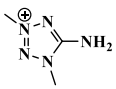
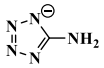
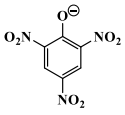
Ionization potential of cations and electron affinity of anions

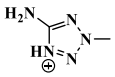
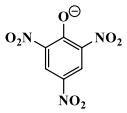
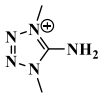
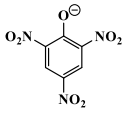
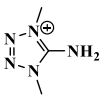
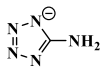
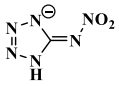
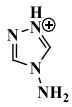
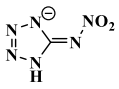
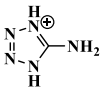
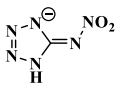
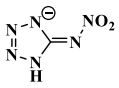
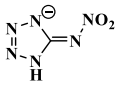
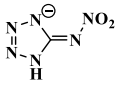
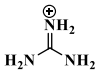
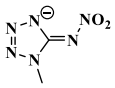
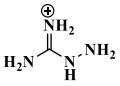
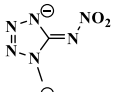
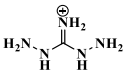
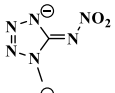
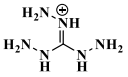
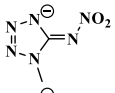
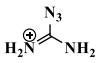
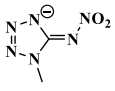
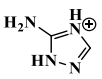
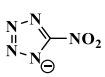
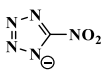
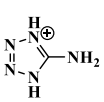
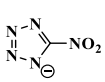
salts	**cation**	**EA(cation)**		**anion**	**IP(anion)**	
		B3LYP/6-311++G(d,p) PCM/water	**B3LYP/aug-cc-pVTZ PCM/water**		**B3LYP/6-311++G(d,p) PCM/water**	**B3LYP/aug-cc-pVTZ PCM/water**
1		1.64	1.64		8.13	8.01
2		1.54	1.54		8.13	8.01
3		1.72	1.71		8.13	8.01
4		1.49	1.48		8.13	8.01
5		1.67	1.65		8.13	8.01
6		0.97	0.99		8.13	8.01
7		1.23	1.24		8.13	8.01
8		1.19	1.20		8.13	8.01
9		1.30	1.30		8.13	8.01
10		1.08	1.07		8.13	8.01

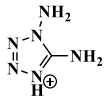
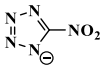
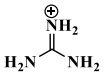
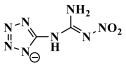
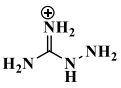
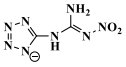
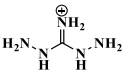
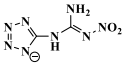
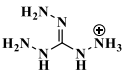
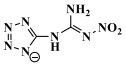
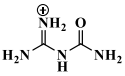
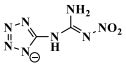
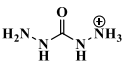
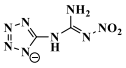
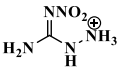
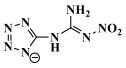
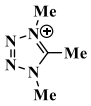
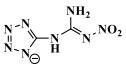
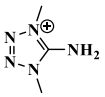
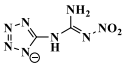
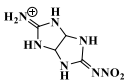
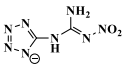
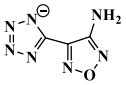
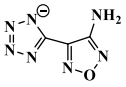
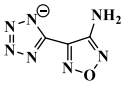
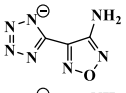
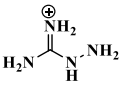
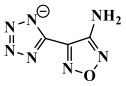
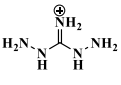
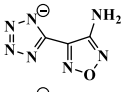
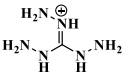
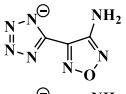
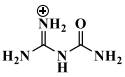
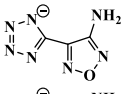
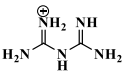
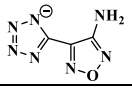
11		1.33	1.30		8.13	8.01
12		2.20	2.16		8.13	8.01
13		3.22	3.15		8.13	8.01
14		1.05	1.05		8.13	8.01
15		1.27	1.27		8.13	8.01
16		2.04	1.99		8.13	8.01
17		2.79	2.76		8.13	8.01
18		1.78	1.75		7.75	7.64
19		1.91	1.87		7.75	7.64
20		1.89	1.86		7.75	7.64
21		2.30	2.19		7.75	7.64
22		1.80	1.76		7.75	7.64
23		1.96	1.91		7.75	7.64
24		1.90	1.86		6.69	6.61
25		1.90	1.86		7.96	7.84
26		2.31	2.21		7.96	7.84
27		2.29	2.21		6.69	6.61

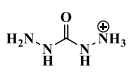
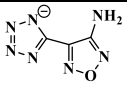
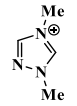
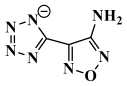
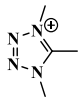
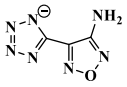
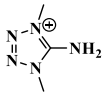
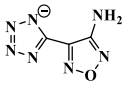
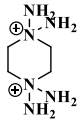
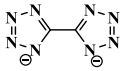
28		1.89	1.85		6.69	6.61
29		1.80	1.77		6.69	6.61
30		2.32	2.21		6.69	6.61
31		2.29	2.19		6.69	6.61
32		1.76	1.72		6.69	6.61
33		1.06	1.05		6.69	6.61
34		1.97	1.92		7.01	6.93
35		2.29	2.21		7.96	7.84
36		1.89	1.85		7.96	7.84
37		1.80	1.77		7.96	7.84
38		2.32	2.21		7.96	7.84
39		2.29	2.19		7.96	7.84
40		2.28	2.18		7.96	7.84
41		1.76	1.72		7.96	7.84
42		1.85	1.81		7.96	7.84

43		2.32	2.21		6.54	6.45
44		1.89	1.85		6.54	6.45
45		1.80	1.77		6.54	6.45
46		1.82	1.79		6.54	6.45
47		2.30	2.19		6.54	6.45
48		0.97	0.97		6.54	6.45
49		1.76	1.72		6.54	6.45
50		1.96	1.91		6.54	6.45
51		2.22	2.18		6.54	6.45
52		2.10	2.07		6.54	6.45
53		2.50	2.45		6.54	6.45
54		1.54	1.53		6.42	6.31
55		3.64	3.56		6.42	6.31
56		1.82	1.79		6.42	6.31

57		2.30	2.19		6.42	6.31
58		1.71	1.67		6.42	6.31
59		1.98	1.93		6.42	6.31
60		2.05	2.01		6.42	6.31
61		1.76	1.72		5.22	5.13
62		1.76	1.72		6.12	6.01
63		1.08	1.07		5.61	5.54
64		1.76	1.72		5.61	5.54
65		1.23	1.24		5.61	5.54
66		1.19	1.20		5.61	5.54
67		1.71	1.67		5.61	5.54
68		1.66	1.63		5.61	5.54
69		1.98	1.93		5.61	5.54
70		1.87	1.83		5.61	5.54
71		2.45	2.39		5.61	5.54
72		1.95	1.91		6.54	6.45

73		2.53	2.46		6.54	6.45
74		1.87	1.83		6.54	6.45
75		1.87	1.83		5.61	5.54
76		1.95	1.91		6.53	6.44
77		1.76	1.72		6.53	6.44
78		1.96	1.91		6.53	6.44
79		1.89	1.85		6.53	6.44
80		1.76	1.72		6.53	6.44
81		2.32	2.22		6.53	6.44
82		1.23	1.24		6.42	6.34
83		1.19	1.20		6.42	6.34
84		1.16	1.96		6.42	6.34
85		1.37	1.38		6.42	6.34
86		2.47	2.38		6.42	6.34
87		0.97	0.97		7.96	7.84
88		2.16	2.11		7.96	7.84
89		1.96	1.91		7.96	7.84

90		2.06	2.00		7.96	7.84
91		1.23	1.24		6.49	6.41
92		1.19	1.20		6.49	6.41
93		1.16	1.96		6.49	6.41
94		1.46	1.46		6.49	6.41
95		1.33	1.30		6.49	6.41
96		1.53	1.51		6.49	6.41
97		2.74	2.64		6.49	6.41
98		2.05	2.01		6.49	6.41
99		1.87	1.83		6.49	6.41
100		2.51	2.41		6.49	6.41
101		1.64	1.64		6.56	6.47
102		1.51	1.49		6.56	6.47
103		1.54	1.54		6.56	6.47
104		1.23	1.24		6.56	6.47
105		1.19	1.20		6.56	6.47
106		1.16	1.96		6.56	6.47
107		1.37	1.38		6.56	6.47
108		1.33	1.30		6.56	6.47
109		1.08	1.07		6.56	6.47

110		1.53	1.51		6.56	6.47
111		1.82	1.79		6.56	6.47
112		2.05	2.01		6.56	6.47
113		1.87	1.83		6.56	6.47
114		1.43	1.42		6.12	6.01
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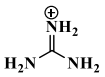
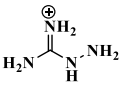
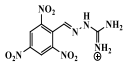
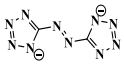
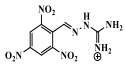
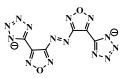
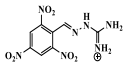
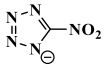
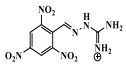
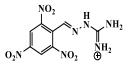
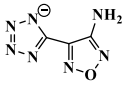
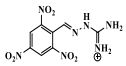
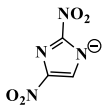
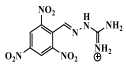
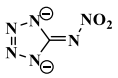
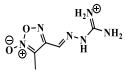
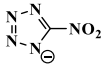
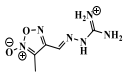
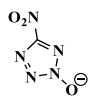
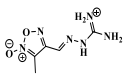
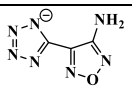
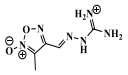
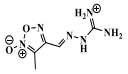
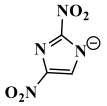
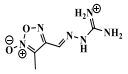
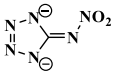
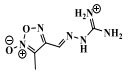
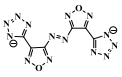
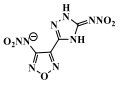
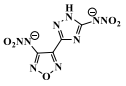
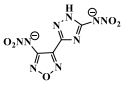
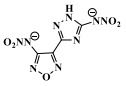
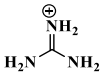
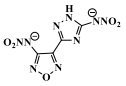
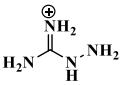
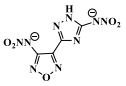
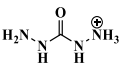
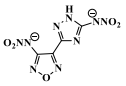
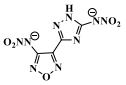
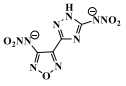
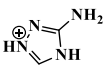
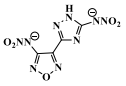
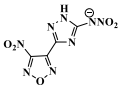
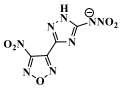
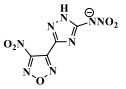
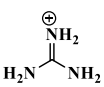
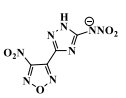
117		1.23	1.24		6.49	6.40
118		1.19	1.20		6.49	6.40
119		4.04	4.16		6.42	6.31
120		4.04	4.16		6.98	6.87
121		4.04	4.16		7.96	7.84
122		4.04	4.16		6.42	6.35
123		4.04	4.16		6.56	6.47
124		4.04	4.16		6.90	6.81
125		4.04	4.16		5.49	5.40
126		3.07	3.02		7.96	7.84
127		3.07	3.02		6.42	6.35

128		3.07	3.02		6.56	6.47
129		3.07	3.02		6.49	6.40
130		3.07	3.02		6.90	6.81
131		3.07	3.02		5.49	5.40
132		3.07	3.02		6.98	6.87
133		1.89	1.85		6.62	6.53
134		1.64	1.64		6.18	6.09
135		1.54	1.54		6.18	6.09
136		1.72	1.71		6.18	6.09
137		1.23	1.24		6.18	6.09
138		1.19	1.20		6.18	6.09
139		1.53	1.51		6.18	6.09
140		1.89	1.85		6.18	6.09
141		1.76	1.72		6.18	6.09
142		1.67	1.63		6.18	6.09
143		1.64	1.64		6.41	6.33
144		1.54	1.54		6.41	6.33
145		1.72	1.71		6.41	6.33
146		1.23	1.24		6.41	6.33

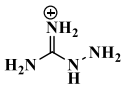
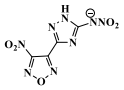
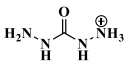
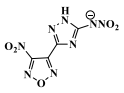
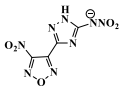
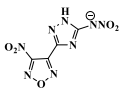
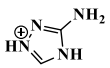
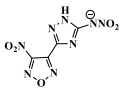
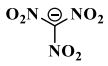
147		1.19	1.20		6.41	6.33
148		1.53	1.51		6.41	6.33
149		1.89	1.85		6.41	6.33
150		1.76	1.72		6.41	6.33
151		1.67	1.63		6.41	6.33
152		1.54	1.54		7.43	7.34

Table S2 Cartesian coordinates of salts

Salt 1

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.00001200	0.00000000	0.00000000
	H2	0.09263200	0.83857300	−0.58434300
	H3	0.10779100	−0.83730900	−0.58355400
	H4	0.72571300	0.00690600	0.72562600
	H5	−0.92605200	−0.00816900	0.44227100
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −56.9203571 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S2: Salt 2

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.65541700	−0.00411800	0.00005100
	N2	−0.75045600	−0.00232700	−0.00003900
	H3	0.99718400	0.96411800	−0.00012100
	H4	1.05415400	−0.45557600	0.83700000
	H5	1.05425800	−0.45589200	−0.83667700
	H6	−1.21844400	−0.89213100	−0.00011000
	H7	−1.22187800	0.88459500	−0.00017400
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −112.2418137 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S3: Salt 3

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.62157632	0.00638917	0.00006179
	O2	−0.73539340	0.09712580	−0.00012371
	H3	1.01706940	0.92485812	−0.00007138
	H4	0.92261491	−0.48604256	0.81669314
	H5	0.92281651	−0.48636615	−0.81629998
	H6	−1.11506675	−0.78460439	0.00000414
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −132.0865145 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S4: Salt 4

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.91505800	0.25420600	0.00009700
	C2	−0.59327600	−0.49095800	−0.00011400
	C3	0.59327600	0.49095800	0.00011400

	N4	1.91505800	−0.25420600	−0.00009700
	H5	−2.69714000	−0.41647900	−0.00005800
	H6	−2.04212000	0.84899600	0.83022300
	H7	−2.04215100	0.84941000	−0.82972700
	H8	−0.59832600	−1.12605500	−0.88826400
	H9	−0.59829300	−1.12650600	0.88771500
	H10	0.59832600	1.12605500	0.88826400
	H11	0.59829300	1.12650600	−0.88771500
	H12	2.69714000	0.41647900	0.00005800
	H13	2.04212000	−0.84899600	−0.83022300
	H14	2.04215100	−0.84941000	0.82972700
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −191.1523481 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S5: Salt 5

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.16382400	−0.67325800	0.00007200
	O2	1.15888500	0.40401800	−0.00000400
	N3	2.48364200	−0.08453600	0.00006000
	C4	−1.25714200	−0.07579200	−0.00001700
	O5	−2.16451800	−0.84597600	0.00008500
	O6	−1.40227400	1.24881900	−0.00019900
	H7	0.27556900	−1.28034500	0.90223800
	H8	0.27561500	−1.28051000	−0.90197700
	H9	3.08891000	0.74710800	−0.00004200
	H10	2.68087600	−0.64340200	0.84494100
	H11	2.68088500	−0.64361400	−0.84467900
	H12	−0.56417700	1.73193800	−0.00028000
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −360.0167181 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S6: Salt 6

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.00000000	0.00000600	0.00000000
	C2	1.23093900	0.87042100	0.00000000
	C3	−1.23094000	0.87042000	0.00000000
	C4	0.00000000	−0.87043100	1.23096600
	C5	0.00000000	−0.87043100	−1.23096600
	H6	2.11354200	0.23304200	0.00000000
	H7	1.22150400	1.49452800	0.89199100
	H8	1.22150400	1.49452800	−0.89199100
	H9	−2.11354200	0.23304200	0.00000000
	H10	−1.22150500	1.49452800	−0.89199000
	H11	−1.22150500	1.49452800	0.89199000
	H12	0.00021300	−0.23302500	2.11354600
	H13	0.89189400	−1.49466900	1.22140400
	H14	−0.89210800	−1.49436600	1.22161700
	H15	0.00021300	−0.23302500	−2.11354600
	H16	−0.89210800	−1.49436600	−1.22161700
	H17	0.89189400	−1.49466900	−1.22140400
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −214.2233642 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S7: Salt 7

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800
	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200

	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S8: Salt 8

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.05049000	−1.92874500	0.00000000
	N2	−0.63398200	−0.66960600	0.00000000
	C3	0.00000000	0.49077800	0.00000000
	N4	−0.71303500	1.63576100	0.00000000
	N5	1.34090500	0.55396100	0.00000000
	H6	−0.67184900	−2.71566800	0.00000000
	H7	0.94319800	−2.04223100	0.00000000
	H8	−1.64306200	−0.68135400	0.00000000
	H9	−0.25481800	2.53243700	0.00000000
	H10	−1.72031300	1.63950200	0.00000000
	H11	1.81372800	1.44388600	0.00000000
	H12	1.92932800	−0.26084100	0.00000000
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S9: Salt 9

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.00000000	2.42944600	−0.09893800
	N2	0.00000000	1.14998700	−0.65450900

	C3	0.00000000	0.00000000	0.02528500
	N4	0.00000000	−1.14998700	−0.65450900
	N5	0.00000000	−2.42944600	−0.09893800
	N6	0.00000000	0.00000000	1.37233500
	H7	0.00000000	3.19851000	−0.74127800
	H8	0.00000000	2.56996300	0.89042200
	H9	0.00000000	1.13876300	−1.66204000
	H10	0.00000000	−1.13876300	−1.66204000
	H11	0.00000000	−3.19851000	−0.74127800
	H12	0.00000000	−2.56996300	0.89042200
	H13	0.00000000	−0.84963300	1.90800300
	H14	0.00000000	0.84963300	1.90800300
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −316.4471704 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S10: Salt 10

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−2.30865200	0.81588200	0.00000000
	C2	−1.21694900	0.03718400	0.00000000
	N3	0.00000000	0.64962600	0.00000000
	C4	1.27171000	0.00451000	0.00000000
	N5	2.30605800	0.88525700	0.00000000
	N6	−1.29726400	−1.27578000	0.00000000
	N7	1.30701300	−1.27093700	0.00000000
	H8	−3.23217400	0.41098800	0.00000000
	H9	−2.25308100	1.82198700	0.00000000
	H10	−0.00498400	1.65842700	0.00000000
	H11	3.25154100	0.53751800	0.00000000
	H12	2.19157500	1.88552200	0.00000000
	H13	−0.38525300	−1.77463900	0.00000000
	H14	−2.18726700	−1.75082900	0.00000000
	H15	2.24099900	−1.66747000	0.00000000
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100

	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −354.7051979 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S11: Salt 11

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	2.31218400	0.76862300	0.00000000
	C2	1.20229600	0.02255600	0.00000000
	N3	0.00000000	0.66359500	0.00000000
	N4	1.26145600	−1.29536300	0.00000000
	C5	−1.27820400	0.00713000	0.00000000
	N6	−2.32216300	0.85491600	0.00000000
	O7	−1.35801900	−1.20338400	0.00000000
	H8	3.22630700	0.34135400	0.00000000
	H9	2.28234200	1.77628500	0.00000000
	H10	0.02372300	1.67372500	0.00000000
	H11	0.37690600	−1.80805400	0.00000000
	H12	2.14512200	−1.78250700	0.00000000
	H13	−3.24569300	0.44611200	0.00000000
	H14	−2.24945800	1.85963800	0.00000000
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −374.5987024 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S12: Salt 12

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	1.75806900	−0.57488600	−0.00004200
	C2	0.75090200	0.29866000	−0.00001000
	N3	3.04773100	−0.13300200	−0.00006300
	C4	−0.61057300	−0.33673600	0.00000800
	N5	−1.59966500	0.63307700	0.00006400
	N6	−2.90571200	0.10701600	0.00005300

	O7	0.85966500	1.52738700	0.00000000
	O8	−0.92031800	−1.51553200	−0.00000500
	H9	1.59160400	−1.57331100	−0.00005100
	H10	3.79088500	−0.80584800	−0.00010800
	H11	3.17878900	0.86522600	−0.00007000
	H12	−1.41787600	1.63278400	0.00005000
	H13	−2.72626200	−0.93289200	0.00000000
	H14	−3.43841300	0.36106800	0.84132500
	H15	−3.43843900	0.36115900	−0.84117500
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −449.709776 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S13: Salt 13

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	4.64460300	−0.37096200	−0.00044300
	O2	3.25611800	−0.58436800	−0.00074100
	C3	2.52993300	0.69044700	0.00071400
	C4	1.04921100	0.39610900	0.00038100
	C5	0.53723900	−0.90192500	0.00052500
	C6	−0.84111500	−1.10432300	0.00032500
	C7	−1.67996700	−0.00034900	0.00002700
	C8	−1.19170200	1.30107300	−0.00009600
	C9	0.18320000	1.49560700	0.00005000
	N10	−3.15315100	−0.21520400	−0.00017500
	O11	−3.85972300	0.78002800	−0.00040700
	O12	−3.54675200	−1.37061900	−0.00003800
	H13	5.06848300	−1.30744800	−0.00141600
	H14	4.95422600	0.13708900	−0.84378600
	H15	4.95413900	0.13530500	0.84400500
	H16	2.82173100	1.24766000	0.89925300
	H17	2.82166600	1.24967900	−0.89658200
	H18	1.19402000	−1.76144200	0.00079700
	H19	−1.26422700	−2.09961600	0.00041100
	H20	−1.88166200	2.13385400	−0.00034000
	H21	0.57351900	2.50792900	−0.00008800

Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −607.073813 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S14: Salt 14

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.50712200	−0.53528200	0.00000000
	N2	−0.56713100	−1.34638000	0.00000000
	N3	−1.73971000	−0.65351600	0.00000000
	C4	−1.38184300	0.59048800	0.00000000
	N5	0.00000000	0.71419300	0.00000000
	N6	0.70444300	1.89288900	0.00000000
	N7	1.80014100	−0.88815100	0.00000000
	H8	−0.58523700	−2.35710100	0.00000000
	H9	−2.05097700	1.43600200	0.00000000
	H10	0.17789700	2.74782300	0.00000000
	H11	1.70633800	1.88155500	0.00000000
	H12	2.54646300	−0.21278800	0.00000000
	H13	2.06964100	−1.85997500	0.00000000
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −353.3810613 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S15: Salt 15

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.60776300	−0.42370200	−0.00090700
	C2	−0.03648700	0.82050400	−0.00617700
	N3	1.31644700	0.57678700	−0.01788400
	C4	1.45163800	−0.82638600	−0.01120500

	N5	0.30139100	−1.47084700	−0.01158900
	C6	−1.94323300	−0.25822900	0.00235500
	N7	−2.09938700	1.08148500	−0.00046200
	N8	−0.89685800	1.79142900	−0.00677900
	N9	2.28479100	1.55951000	0.02345500
	N10	2.65887200	−1.40721700	0.03767200
	N11	−2.86076400	−1.22861600	0.01233500
	H12	−2.96413300	1.60239100	0.00883900
	H13	2.83875100	1.53061600	0.87133500
	H14	2.82928700	1.61557700	−0.82886500
	H15	2.70933100	−2.41271800	−0.02969500
	H16	3.49074100	−0.88102600	−0.17671300
	H17	−3.84768700	−1.02850500	−0.00868100
	H18	−2.56489700	−2.19347000	0.00305200
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −556.4008576 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S16: Salt 16

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−2.36597700	−1.56459900	0.00000500
	C2	−2.85380700	−0.32148600	0.00000300
	N3	−1.83383700	0.58129700	−0.00000300
	C4	−0.69199400	−0.18874700	−0.00000300
	N5	−1.02574000	−1.47083200	0.00000200
	N6	−4.16968300	−0.01110300	0.00000300
	C7	0.65231300	0.29383200	0.00000000
	N8	1.05072300	1.54373000	0.00000500
	N9	2.41535300	1.46842300	0.00000500
	C10	2.85382700	0.19737000	0.00000000
	N11	1.74893800	−0.57062000	−0.00000100
	N12	−1.90491700	1.95699400	−0.00002500
	N13	1.67092700	−1.93908100	−0.00000300
	N14	4.12649300	−0.22950300	−0.00000100
	H15	−4.82868300	−0.77277200	0.00000300
	H16	−4.52781600	0.92607700	0.00000700

	H17	2.96473700	2.31497400	0.00000700
	H18	−2.80467200	2.39575300	0.00002400
	H19	−1.03638400	2.46348700	0.00007300
	H20	0.71532600	−2.30403300	−0.00000200
	H21	2.51498000	−2.47926000	−0.00000900
	H22	4.36191900	−1.20780100	−0.00000400
	H23	4.89260200	0.42480700	0.00000000
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −705.2135034 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S17: Salt 17

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−2.76619800	−0.04963200	0.00089200
	N2	−2.75984000	−1.33372300	0.40073900
	N3	−1.50077000	−1.87154300	0.45055700
	C4	−0.72367600	−0.91568500	0.06460000
	N5	−1.45002000	0.25318900	−0.20725900
	N6	−3.78002900	0.77491400	−0.17698600
	C7	0.72362900	−0.91569600	−0.06428900
	N8	1.50060900	−1.87154300	−0.45054600
	N9	2.75970400	−1.33381800	−0.40082600
	C10	2.76618200	−0.04971800	−0.00099200
	N11	1.45007400	0.25311600	0.20751500
	N12	3.78006800	0.77483700	0.17657400
	N13	−0.98754100	1.43355200	−0.77716800
	C14	−0.00001200	2.20388400	0.00008100
	N15	0.98777300	1.43360000	0.77721100
	H16	−3.54944100	−1.91639600	0.65767800
	H17	−3.60678500	1.70716000	−0.53312400
	H18	−4.73954900	0.48830400	−0.03444200
	H19	3.54926900	−1.91658800	−0.65765700
	H20	3.60695100	1.70698000	0.53304700
	H21	4.73953100	0.48827800	0.03355400
	H22	−0.70666700	1.26518300	−1.73907900
	H23	0.49793700	2.84245900	−0.73074300

	H24	−0.49812100	2.84212100	0.73109200
	H25	0.70714500	1.26552200	1.73924100
Anion	N1	1.09782300	−0.25964600	0.00008600
	N2	0.58607900	0.96336400	−0.00000300
	N3	−0.73534900	0.85500500	−0.00008100
	N4	−1.04076500	−0.43504700	0.00013400
	N5	0.09221200	−1.12367700	−0.00013600

SCF Done: E(B3LYP, cation) = −743.608022 a.u.

SCF Done: E(B3LYP, anion) = −273.8228097 a.u.

Table S18: Salt 18

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.95998000	1.08037900	0.00004000
	N2	−0.74863600	1.56336400	0.00001600
	N3	0.06046900	0.47142700	−0.00004600
	C4	−0.65089200	−0.64528600	−0.00017800
	N5	−1.94883600	−0.29194300	−0.00002700
	C6	−3.11298100	−1.19686300	0.00008600
	C7	3.81669700	−0.39891300	0.00006300
	C8	2.30519100	−0.65934400	0.00004000
	C9	1.53314100	0.65473400	−0.00004000
	H10	−2.86086800	1.67373700	0.00012300
	H11	−0.26884000	−1.65229700	−0.00030400
	H12	−4.01466800	−0.58833100	0.00008800
	H13	−3.09629700	−1.81745400	−0.89494700
	H14	−3.09622100	−1.81735500	0.89518800
	H15	4.36083800	−1.34425700	0.00012200
	H16	4.12464500	0.16268700	−0.88520800
	H17	4.12460300	0.16277200	0.88529600
	H18	2.04010400	−1.24873200	0.88485900
	H19	2.04015200	−1.24881800	−0.88473600
	H20	1.75926500	1.25488300	−0.88340000
	H21	1.75925200	1.25498800	0.88325100
Anion	N1	−0.66794700	−1.46327300	−0.00018400
	C2	−1.01162700	−0.16002100	0.00007000
	N3	−0.00000100	0.70958100	0.00031400
	C4	1.01162700	−0.16002300	0.00014800
	N5	0.66796000	−1.46327800	0.00043900
	N6	−2.40065100	0.26300100	−0.00000300
	O7	−3.26725400	−0.60961200	−0.00035500

	O8	−2.63610000	1.46942000	0.00013900
	N9	2.40064900	0.26300400	−0.00012800
	O10	2.63608900	1.46942400	−0.00020900
	O11	3.26725500	−0.60960600	−0.00012200

SCF Done: E(B3LYP, cation) = −399.9844557 a.u.

SCF Done: E(B3LYP, anion) = −650.9218673 a.u.

Table S19: Salt 19

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	2.87140500	−0.88054800	−0.00055200
	N2	1.74972100	−1.54544900	0.00034800
	N3	0.78140300	−0.59207600	0.00019000
	C4	1.31251200	0.62241300	0.00070400
	N5	2.64831200	0.47329200	−0.00004300
	C6	3.65971500	1.54792600	−0.00019800
	C7	−0.63314800	−1.01825800	0.00005800
	C8	−1.60874400	0.15515800	−0.00004600
	N9	−2.93234200	−0.47322400	−0.00014300
	N10	−3.89400400	0.30831600	−0.00012000
	N11	−4.85266100	0.90457100	−0.00011000
	H12	3.85274600	−1.32859400	−0.00111200
	H13	0.78368200	1.56121400	0.00116100
	H14	4.64407400	1.08517200	−0.00101400
	H15	3.54643000	2.15804800	−0.89529600
	H16	3.54753800	2.15728000	0.89556300
	H17	−0.77820900	−1.63921600	0.88444600
	H18	−0.77808600	−1.63927000	−0.88431300
	H19	−1.46573100	0.77858400	−0.89304500
	H20	−1.46588400	0.77862600	0.89294800
Anion	N1	−0.66794700	−1.46327300	−0.00018400
	C2	−1.01162700	−0.16002100	0.00007000
	N3	−0.00000100	0.70958100	0.00031400
	C4	1.01162700	−0.16002300	0.00014800
	N5	0.66796000	−1.46327800	0.00043900
	N6	−2.40065100	0.26300100	−0.00000300
	O7	−3.26725400	−0.60961200	−0.00035500
	O8	−2.63610000	1.46942000	0.00013900
	N9	2.40064900	0.26300400	−0.00012800
	O10	2.63608900	1.46942400	−0.00020900
	O11	3.26725500	−0.60960600	−0.00012200

SCF Done: E(B3LYP, cation) = −524.2704084 a.u.
SCF Done: E(B3LYP, anion) = −650.9218673 a.u.

Table S20: Salt 20

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.09878300	1.10871700	−0.00090000
	N2	−2.39547400	1.25769000	−0.00096500
	N3	−2.88786000	−0.00653400	0.00039300
	C4	−1.90913800	−0.89798900	−0.00035000
	N5	−0.74840800	−0.22007700	−0.00087900
	C6	0.60181300	−0.84175200	−0.00148600
	C7	1.72874200	0.18909300	0.00021400
	N8	2.94961000	−0.62150000	−0.00032300
	N9	4.01357700	0.01498300	0.00061800
	N10	5.04752200	0.46730400	0.00136000
	C11	−4.33852600	−0.23320300	0.00187100
	H12	−0.39638400	1.92535400	−0.00137100
	H13	−2.01832000	−1.97091800	−0.00007500
	H14	0.68153100	−1.46967200	−0.88954900
	H15	0.68113600	−1.47206100	0.88491400
	H16	1.67130600	0.82437900	0.89343000
	H17	1.67202000	0.82657700	−0.89147900
	H18	−4.52389900	−1.30550300	0.00242000
	H19	−4.76158200	0.22511000	0.89436500
	H20	−4.76321300	0.22446800	−0.89017200
Anion	N1	−0.66794700	−1.46327300	−0.00018400
	C2	−1.01162700	−0.16002100	0.00007000
	N3	−0.00000100	0.70958100	0.00031400
	C4	1.01162700	−0.16002300	0.00014800
	N5	0.66796000	−1.46327800	0.00043900
	N6	−2.40065100	0.26300100	−0.00000300
	O7	−3.26725400	−0.60961200	−0.00035500
	O8	−2.63610000	1.46942000	0.00013900
	N9	2.40064900	0.26300400	−0.00012800
	O10	2.63608900	1.46942400	−0.00020900
	O11	3.26725500	−0.60960600	−0.00012200

SCF Done: E(B3LYP, cation) = −524.2708654 a.u.
SCF Done: E(B3LYP, anion) = −650.9218673 a.u.

Table S21: Salt 21

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.18477700	−0.48806600	−0.00017100
	N2	−0.95937800	−1.14105000	−0.00018500
	N3	−1.91196800	−0.18023500	0.00005300
	C4	−1.38445400	1.02649200	0.00005300
	N5	−0.04134400	0.88642500	−0.00005800
	C6	0.89524300	2.03075200	−0.00012200
	C7	−3.32873300	−0.56230300	0.00021500
	N8	1.34903900	−1.20352600	−0.00035600
	N9	2.47345600	−0.67220400	0.00009700
	N10	3.56526000	−0.39981600	0.00040300
	H11	−1.91807500	1.96378500	0.00016800
	H12	1.91877100	1.67476400	−0.00053300
	H13	0.73147200	2.62963000	−0.89531300
	H14	0.73204600	2.62928600	0.89540500
	H15	−3.93391500	0.34219600	0.00043500
	H16	−3.52851500	−1.15391500	−0.89190000
	H17	−3.52824900	−1.15417100	0.89221900
Anion	N1	−0.66794700	−1.46327300	−0.00018400
	C2	−1.01162700	−0.16002100	0.00007000
	N3	−0.00000100	0.70958100	0.00031400
	C4	1.01162700	−0.16002300	0.00014800
	N5	0.66796000	−1.46327800	0.00043900
	N6	−2.40065100	0.26300100	−0.00000300
	O7	−3.26725400	−0.60961200	−0.00035500
	O8	−2.63610000	1.46942000	0.00013900
	N9	2.40064900	0.26300400	−0.00012800
	O10	2.63608900	1.46942400	−0.00020900
	O11	3.26725500	−0.60960600	−0.00012200

SCF Done: E(B3LYP, cation) = −484.9450554 a.u.

SCF Done: E(B3LYP, anion) = −650.9218673 a.u.

Table S22: Salt 22

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	2.89223000	−0.84681300	−0.00007600
	N2	1.76828200	−1.51421700	−0.00001800
	N3	0.79660100	−0.58247900	0.00009300

	C4	1.31177700	0.64987800	0.00011300
	N5	2.64710500	0.50518900	0.00000300
	N6	3.58043400	1.49862900	−0.00002800
	C7	−0.61547700	−1.01884600	0.00021400
	C8	−1.59780800	0.14905600	−0.00009200
	N9	−2.91800400	−0.48602400	−0.00001700
	N10	−3.88380400	0.29003300	−0.00007800
	N11	−4.84616700	0.88045200	−0.00012200
	H12	3.87888200	−1.28201500	−0.00017500
	H13	0.77753900	1.58442500	0.00019900
	H14	4.54962400	1.23410500	−0.00012000
	H15	3.27341800	2.45497100	0.00003500
	H16	−0.75866400	−1.63903700	0.88546900
	H17	−0.75865400	−1.63948000	−0.88473100
	H18	−1.45875200	0.77294300	−0.89346700
	H19	−1.45884600	0.77335200	0.89301100
Anion	N1	−0.66794700	−1.46327300	−0.00018400
	C2	−1.01162700	−0.16002100	0.00007000
	N3	−0.00000100	0.70958100	0.00031400
	C4	1.01162700	−0.16002300	0.00014800
	N5	0.66796000	−1.46327800	0.00043900
	N6	−2.40065100	0.26300100	−0.00000300
	O7	−3.26725400	−0.60961200	−0.00035500
	O8	−2.63610000	1.46942000	0.00013900
	N9	2.40064900	0.26300400	−0.00012800
	O10	2.63608900	1.46942400	−0.00020900
	O11	3.26725500	−0.60960600	−0.00012200

SCF Done: E(B3LYP, cation) = −540.2671406 a.u.

SCF Done: E(B3LYP, anion) = −650.9218673 a.u.

Table S23: Salt 23

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.59742900	−1.53950800	−0.00004700
	N2	−0.66881200	−1.53321300	0.00000800
	N3	−1.07173000	−0.22648800	0.00002800
	C4	−0.00603900	0.58942200	−0.00002500
	N5	1.03461400	−0.24552600	−0.00008400
	N6	−2.39402200	0.18054700	0.00004600
	C7	−0.00401400	2.06752800	−0.00001300
	C8	2.47346300	0.05182800	0.00006500

	H9	−2.85710600	−0.17504600	−0.83326500
	H10	−2.85715400	−0.17540200	0.83317800
	H11	0.51462100	2.44501700	−0.88550100
	H12	−1.02999200	2.43188900	0.00025000
	H13	0.51505600	2.44498800	0.88523500
	H14	2.99048900	−0.90499400	−0.00023500
	H15	2.73067200	0.61539500	−0.89632800
	H16	2.73060000	0.61480100	0.89685300
Anion	N1	−0.66794700	−1.46327300	−0.00018400
	C2	−1.01162700	−0.16002100	0.00007000
	N3	−0.00000100	0.70958100	0.00031400
	C4	1.01162700	−0.16002300	0.00014800
	N5	0.66796000	−1.46327800	0.00043900
	N6	−2.40065100	0.26300100	−0.00000300
	O7	−3.26725400	−0.60961200	−0.00035500
	O8	−2.63610000	1.46942000	0.00013900
	N9	2.40064900	0.26300400	−0.00012800
	O10	2.63608900	1.46942400	−0.00020900
	O11	3.26725500	−0.60960600	−0.00012200

SCF Done: E(B3LYP, cation) = −392.6831906 a.u.

SCF Done: E(B3LYP, anion) = −650.9218673 a.u.

Table S24: Salt 24

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	3.35468900	−0.29963400	0.00002900
	N2	2.31701600	−1.08583400	−0.00013900
	N3	1.23834300	−0.25134200	0.00000300
	C4	1.61519900	1.01603600	−0.00010100
	N5	2.95905600	1.01426000	0.00006400
	C6	−0.11531200	−0.84712800	0.00011600
	C7	−1.22721400	0.19790700	−0.00003800
	N8	−2.46118600	−0.59117300	0.00000800
	N9	−3.51346600	0.06445600	0.00000200
	N10	−4.53954000	0.53461700	0.00000100
	H11	4.38281200	−0.62629100	0.00006900
	H12	0.98218700	1.88791900	−0.00015500
	H13	3.55525000	1.83419200	0.00029900
	H14	−0.18057000	−1.48111300	0.88483800
	H15	−0.18056400	−1.48135200	−0.88443300
	H16	−1.16238800	0.83422900	−0.89330800

	H17	−1.16245200	0.83443800	0.89308700
Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700
	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −484.9431898 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S25: Salt 25

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	3.35468900	−0.29963400	0.00002900
	N2	2.31701600	−1.08583400	−0.00013900
	N3	1.23834300	−0.25134200	0.00000300
	C4	1.61519900	1.01603600	−0.00010100
	N5	2.95905600	1.01426000	0.00006400
	C6	−0.11531200	−0.84712800	0.00011600
	C7	−1.22721400	0.19790700	−0.00003800
	N8	−2.46118600	−0.59117300	0.00000800
	N9	−3.51346600	0.06445600	0.00000200
	N10	−4.53954000	0.53461700	0.00000100
	H11	4.38281200	−0.62629100	0.00006900
	H12	0.98218700	1.88791900	−0.00015500
	H13	3.55525000	1.83419200	0.00029900
	H14	−0.18057000	−1.48111300	0.88483800
	H15	−0.18056400	−1.48135200	−0.88443300
	H16	−1.16238800	0.83422900	−0.89330800
	H17	−1.16245200	0.83443800	0.89308700
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000

	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −484.9431898 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S26: Salt 26

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	2.14463400	−0.30409000	0.00000000
	N2	1.08918100	−1.08486500	0.00003300
	N3	0.02309400	−0.23779200	0.00006700
	C4	0.39886900	1.02440800	0.00008400
	N5	1.74898300	1.02511000	0.00001600
	N6	3.41271400	−0.80956000	−0.00007700
	N7	4.37229100	−0.00859800	−0.00004700
	N8	5.34128000	0.56030400	−0.00004300
	C9	−1.33172400	−0.82827600	0.00009500
	C10	−2.44067200	0.21969900	−0.00003200
	N11	−3.67761500	−0.56532300	−0.00002900
	N12	−4.72730800	0.09390800	−0.00004300
	N13	−5.75155400	0.56833300	−0.00005600
	H14	−0.23101400	1.89855300	0.00010800
	H15	2.33162100	1.85408200	0.00011600
	H16	−1.39790900	−1.46273100	0.88444200
	H17	−1.39786600	−1.46289200	−0.88413900
	H18	−2.37442600	0.85589100	−0.89317900
	H19	−2.37450800	0.85602900	0.89302200
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −648.5639247 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S27: Salt 27

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.91162800	1.01660900	−0.00000500
	C2	2.33196700	−0.26931200	0.00000900
	N3	1.19384000	−1.06547000	−0.00000100
	C4	0.09727700	−0.29383100	−0.00000300
	N5	0.51721300	0.98561500	0.00000100
	N6	−1.14891600	−0.84019600	−0.00000700
	N7	−2.13984200	−0.07334800	0.00000100
	N8	−3.12429200	0.46490500	0.00000600
	H9	2.46023100	1.94259000	−0.00001000
	H10	3.32336300	−0.68820900	0.00001500
	H11	1.16522900	−2.07783300	0.00000300
	H12	−0.08007400	1.80211500	−0.00000100
Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700
	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −390.2793719 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S28: Salt 28

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.06640500	−0.41832800	−0.00003200
	N2	0.03611200	−1.21412900	−0.00000400
	N3	−1.03285300	−0.37700300	0.00003700
	C4	−0.67974900	0.89734900	−0.00005800
	N5	0.65865300	0.89769800	0.00002500
	H6	2.09788600	−0.73449200	−0.00004900
	H7	−1.97156900	−0.76356700	0.00008100
	H8	−1.33192900	1.75728600	−0.00010100

	H9	1.25228900	1.72069000	0.00019900
Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700
	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −242.6694066 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S29: Salt 29

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.34395300	−0.76133900	−0.00002500
	N2	−0.09641400	−1.13546600	0.00009700
	N3	0.61937000	0.02363800	−0.00000100
	C4	−0.17515000	1.07971800	0.00011100
	N5	−1.43290700	0.60853900	−0.00005400
	C6	2.08835000	−0.02286700	−0.00006700
	H7	−2.19345800	−1.42615900	−0.00006900
	H8	0.12266600	2.11627900	0.00017900
	H9	−2.27850900	1.16781500	−0.00027500
	H10	2.46870200	0.99662400	−0.00024600
	H11	2.41742300	−0.55216200	0.89275000
	H12	2.41735100	−0.55244700	−0.89274100
Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700

	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −282.0020614 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S30: Salt 30

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.10928300	−0.37050500	−0.00001000
	N2	1.16549400	−1.15216600	−0.00009000
	N3	2.21450300	−0.29340200	0.00006400
	C4	1.85243700	0.97271400	−0.00003500
	N5	0.50786700	0.96531600	0.00002000
	N6	−1.15653700	−0.87371600	0.00003400
	N7	−2.11886300	−0.07468100	0.00000600
	N8	−3.09035500	0.48886000	0.00000100
	H9	3.15781300	−0.66781200	0.00015800
	H10	2.49471700	1.83993100	−0.00001900
	H11	−0.07760900	1.79315200	−0.00011500
Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700
	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −406.2900901 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S31: Salt 31

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.32893900	−0.28721400	0.00001400
	N2	0.79794200	−0.96170600	0.00000800

	N3	1.77356600	−0.01366000	−0.00001900
	C4	1.27830400	1.20574900	0.00001500
	N5	−0.06489500	1.07521800	0.00004500
	N6	−1.54183000	−0.91313700	0.00004800
	N7	−2.57474900	−0.20924800	−0.00001300
	N8	−3.59430700	0.26297300	−0.00004500
	C9	3.18197800	−0.42974100	−0.00002900
	H10	1.82897400	2.13304200	0.00003700
	H11	−0.72595600	1.84313500	−0.00010900
	H12	3.80813200	0.46031100	−0.00018500
	H13	3.36539900	−1.02604800	0.89239800
	H14	3.36530300	−1.02629200	−0.89231100
Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700
	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −445.6228493 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S32: Salt 32

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.72573800	−1.43573300	0.00000000
	C2	1.10022700	−0.18529000	0.00000000
	N3	0.00000000	0.65115400	0.00000000
	C4	−1.08228900	−0.13710400	0.00000000
	N5	−0.61573600	−1.38850300	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	2.12050200	0.16391300	0.00000000
	H8	−2.11338600	0.17676100	0.00000000
	H9	−1.15210300	−2.24869500	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000

Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700
	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S33: Salt 33

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.21497100	0.71391700	−0.00002900
	N2	−0.31228300	−0.62561700	−0.00019000
	N3	0.92846700	−1.23600100	−0.00004200
	C4	1.76605100	−0.25487100	0.00003500
	N5	1.11344200	0.97170900	0.00022200
	N6	−1.23484900	1.56243700	0.00002300
	N7	−1.52533600	−1.28624200	0.00006300
	H8	2.84023500	−0.35221900	0.00017300
	H9	1.54903700	1.88443600	−0.00106700
	H10	−2.17216900	1.18116500	−0.00010400
	H11	−1.10937000	2.56245200	0.00013800
	H12	−1.60005800	−1.86694400	0.83220300
	H13	−1.60024000	−1.86717100	−0.83190300
Anion	C1	0.79717000	0.28342400	0.00000900
	C2	−0.58056800	0.53786700	0.00000200
	N3	−0.81036200	1.84623700	0.00000200
	C4	0.45875900	2.35802000	−0.00000800
	N5	1.45163600	1.47525100	0.00000500
	N6	1.44641200	−0.97668100	0.00001400
	O7	0.72010200	−1.98641900	−0.00001300
	O8	2.67855900	−1.02697400	−0.00000700
	N9	−1.71005700	−0.40124600	0.00000100
	O10	−2.15717700	−0.75001000	1.08450700

	O11	−2.15718700	−0.74999700	−1.08450600
	H12	0.63005500	3.42640600	−0.00001000

SCF Done: E(B3LYP, cation) = −353.414357 a.u.

SCF Done: E(B3LYP, anion) = −634.882769 a.u.

Table S34: Salt 34

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.30897900	−0.76354400	0.00027600
	N2	0.05235900	−1.13072300	−0.00042700
	N3	−0.64226500	0.03501800	−0.00008200
	C4	0.15440800	1.09354800	−0.00026700
	N5	1.41502700	0.59184600	0.00011800
	N6	−1.98939000	−0.02302000	−0.00005200
	H7	2.14407700	−1.44581400	0.00053200
	H8	−0.13228000	2.13167200	−0.00047700
	H9	2.26724800	1.13951000	0.00045500
	H10	−2.38904500	−0.94767400	0.00093900
	H11	−2.52043400	0.83044200	0.00159200
Anion	C1	0.06990000	0.00372200	0.00003400
	N2	0.77179900	−1.13794900	0.00010800
	N3	2.05955200	−0.74304900	−0.00007000
	C4	2.02817300	0.60943000	−0.00009400
	N5	0.79932800	1.13670200	0.00014500
	N6	−1.37056900	0.01090600	−0.00006900
	O7	−1.95075800	1.10172600	−0.00002400
	O8	−1.96690600	−1.07057200	−0.00001100
	H9	2.93210800	1.20559000	−0.00015700

SCF Done: E(B3LYP, cation) = −298.0042867 a.u.

SCF Done: E(B3LYP, anion) = −446.3474789 a.u.

Table S35: Salt 35

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.91162800	1.01660900	−0.00000500
	C2	2.33196700	−0.26931200	0.00000900
	N3	1.19384000	−1.06547000	−0.00000100
	C4	0.09727700	−0.29383100	−0.00000300
	N5	0.51721300	0.98561500	0.00000100

	N6	−1.14891600	−0.84019600	−0.00000700
	N7	−2.13984200	−0.07334800	0.00000100
	N8	−3.12429200	0.46490500	0.00000600
	H9	2.46023100	1.94259000	−0.00001000
	H10	3.32336300	−0.68820900	0.00001500
	H11	1.16522900	−2.07783300	0.00000300
	H12	−0.08007400	1.80211500	−0.00000100
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −390.2793719 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S36: Salt 36

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.06640500	−0.41832800	−0.00003200
	N2	0.03611200	−1.21412900	−0.00000400
	N3	−1.03285300	−0.37700300	0.00003700
	C4	−0.67974900	0.89734900	−0.00005800
	N5	0.65865300	0.89769800	0.00002500
	H6	2.09788600	−0.73449200	−0.00004900
	H7	−1.97156900	−0.76356700	0.00008100
	H8	−1.33192900	1.75728600	−0.00010100
	H9	1.25228900	1.72069000	0.00019900
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −242.6694066 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S37: Salt 37

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.34395300	−0.76133900	−0.00002500
	N2	−0.09641400	−1.13546600	0.00009700
	N3	0.61937000	0.02363800	−0.00000100
	C4	−0.17515000	1.07971800	0.00011100
	N5	−1.43290700	0.60853900	−0.00005400
	C6	2.08835000	−0.02286700	−0.00006700
	H7	−2.19345800	−1.42615900	−0.00006900
	H8	0.12266600	2.11627900	0.00017900
	H9	−2.27850900	1.16781500	−0.00027500
	H10	2.46870200	0.99662400	−0.00024600
	H11	2.41742300	−0.55216200	0.89275000
	H12	2.41735100	−0.55244700	−0.89274100
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −282.0020614 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S38: Salt 38

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.10928300	−0.37050500	−0.00001000
	N2	1.16549400	−1.15216600	−0.00009000
	N3	2.21450300	−0.29340200	0.00006400
	C4	1.85243700	0.97271400	−0.00003500
	N5	0.50786700	0.96531600	0.00002000
	N6	−1.15653700	−0.87371600	0.00003400
	N7	−2.11886300	−0.07468100	0.00000600
	N8	−3.09035500	0.48886000	0.00000100
	H9	3.15781300	−0.66781200	0.00015800
	H10	2.49471700	1.83993100	−0.00001900

	H11	−0.07760900	1.79315200	−0.00011500
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −406.2900901 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S39: Salt 39

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.32893900	−0.28721400	0.00001400
	N2	0.79794200	−0.96170600	0.00000800
	N3	1.77356600	−0.01366000	−0.00001900
	C4	1.27830400	1.20574900	0.00001500
	N5	−0.06489500	1.07521800	0.00004500
	N6	−1.54183000	−0.91313700	0.00004800
	N7	−2.57474900	−0.20924800	−0.00001300
	N8	−3.59430700	0.26297300	−0.00004500
	C9	3.18197800	−0.42974100	−0.00002900
	H10	1.82897400	2.13304200	0.00003700
	H11	−0.72595600	1.84313500	−0.00010900
	H12	3.80813200	0.46031100	−0.00018500
	H13	3.36539900	−1.02604800	0.89239800
	H14	3.36530300	−1.02629200	−0.89231100
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −445.6228493 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S40: Salt 40

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.34509800	−0.32050900	−0.00003300
	N2	0.25046700	−1.04397700	−0.00005000
	N3	−0.76958100	−0.14153200	−0.00008300
	C4	−0.32773300	1.09779800	−0.00012800
	N5	1.02139600	1.02768800	−0.00010900
	N6	2.58684200	−0.89120000	−0.00000800
	N7	3.58509200	−0.14026000	0.00008400
	N8	4.58098200	0.38086700	0.00014900
	C9	−4.62478600	−0.11455300	0.00013300
	C10	−3.20701000	0.47166300	0.00011300
	C11	−2.16740600	−0.64221800	−0.00010900
	H12	−0.91486000	2.00082900	−0.00019000
	H13	1.64705500	1.82428500	0.00005700
	H14	−5.36295900	0.68832100	0.00027200
	H15	−4.80147900	−0.72997800	−0.88518500
	H16	−4.80136900	−0.73018400	0.88533000
	H17	−3.07768000	1.10408400	0.88534900
	H18	−3.07781400	1.10432400	−0.88497100
	H19	−2.25317000	−1.27779800	−0.88345200
	H20	−2.25308400	−1.27807200	0.88304500
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −524.2783429 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S41: Salt 41

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.72573800	−1.43573300	0.00000000
	C2	1.10022700	−0.18529000	0.00000000
	N3	0.00000000	0.65115400	0.00000000

	C4	−1.08228900	−0.13710400	0.00000000
	N5	−0.61573600	−1.38850300	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	2.12050200	0.16391300	0.00000000
	H8	−2.11338600	0.17676100	0.00000000
	H9	−1.15210300	−2.24869500	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S42: Salt 42

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−3.29840800	−0.93880500	0.00023200
	N2	−3.67320100	0.38678800	0.00000300
	C3	−2.59258100	1.10884400	−0.00017900
	N4	−1.48703500	0.28376600	−0.00003400
	C5	−1.99731800	−1.00216200	−0.00007300
	N6	2.20576300	0.49271600	0.00002900
	C7	0.91583700	−0.03675700	0.00000500
	N8	0.94704000	−1.35546600	−0.00004200
	N9	2.27850800	−1.64309600	−0.00003300
	C10	3.03472800	−0.56805900	−0.00003400
	N11	−0.17454100	0.74888300	0.00003200
	C12	2.58513300	1.91320700	0.00008000
	H13	−2.53737700	2.18737300	−0.00028200
	H14	−1.39086800	−1.88959800	−0.00003900
	H15	2.57539500	−2.61215300	−0.00004900
	H16	4.11278100	−0.53272700	−0.00004500
	H17	−0.08978200	1.75336500	0.00004300
	H18	3.67062100	1.98538300	0.00010200
	H19	2.19878900	2.39723600	−0.89828400

	H20	2.19875600	2.39718200	0.89845900
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −578.4101108 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S43: Salt 43

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.10928300	−0.37050500	−0.00001000
	N2	1.16549400	−1.15216600	−0.00009000
	N3	2.21450300	−0.29340200	0.00006400
	C4	1.85243700	0.97271400	−0.00003500
	N5	0.50786700	0.96531600	0.00002000
	N6	−1.15653700	−0.87371600	0.00003400
	N7	−2.11886300	−0.07468100	0.00000600
	N8	−3.09035500	0.48886000	0.00000100
	H9	3.15781300	−0.66781200	0.00015800
	H10	2.49471700	1.83993100	−0.00001900
	H11	−0.07760900	1.79315200	−0.00011500
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400

	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −406.2900901 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S44: Salt 44

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.06640500	−0.41832800	−0.00003200
	N2	0.03611200	−1.21412900	−0.00000400
	N3	−1.03285300	−0.37700300	0.00003700
	C4	−0.67974900	0.89734900	−0.00005800
	N5	0.65865300	0.89769800	0.00002500
	H6	2.09788600	−0.73449200	−0.00004900
	H7	−1.97156900	−0.76356700	0.00008100
	H8	−1.33192900	1.75728600	−0.00010100
	H9	1.25228900	1.72069000	0.00019900
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −242.6694066 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S45: Salt 45

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.34395300	−0.76133900	−0.00002500
	N2	−0.09641400	−1.13546600	0.00009700
	N3	0.61937000	0.02363800	−0.00000100
	C4	−0.17515000	1.07971800	0.00011100
	N5	−1.43290700	0.60853900	−0.00005400
	C6	2.08835000	−0.02286700	−0.00006700
	H7	−2.19345800	−1.42615900	−0.00006900
	H8	0.12266600	2.11627900	0.00017900
	H9	−2.27850900	1.16781500	−0.00027500
	H10	2.46870200	0.99662400	−0.00024600
	H11	2.41742300	−0.55216200	0.89275000
	H12	2.41735100	−0.55244700	−0.89274100
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −282.0020614 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S46: Salt 46

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.59451600	1.20187700	−0.00003200
	N2	0.70987100	1.21521700	−0.00001400

	N3	1.06725400	−0.09451300	0.00000000
	C4	0.00077400	−0.88021700	−0.00013000
	N5	−1.08025000	−0.08242400	−0.00002500
	C6	−2.49413600	−0.50489600	0.00008000
	C7	2.48650600	−0.47089700	0.00007100
	H8	−1.22032700	2.08055400	−0.00001100
	H9	−0.00234600	−1.95863900	−0.00020400
	H10	−3.11391800	0.38900000	0.00000800
	H11	−2.70184400	−1.08933900	−0.89524100
	H12	−2.70178700	−1.08916200	0.89553200
	H13	2.55902600	−1.55669300	0.00020400
	H14	2.95566400	−0.05954800	−0.89231300
	H15	2.95564100	−0.05933200	0.89236600
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −321.329351 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S47: Salt 47

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.18477700	−0.48806600	−0.00017100
	N2	−0.95937800	−1.14105000	−0.00018500
	N3	−1.91196800	−0.18023500	0.00005300
	C4	−1.38445400	1.02649200	0.00005300

	N5	−0.04134400	0.88642500	−0.00005800
	C6	0.89524300	2.03075200	−0.00012200
	C7	−3.32873300	−0.56230300	0.00021500
	N8	1.34903900	−1.20352600	−0.00035600
	N9	2.47345600	−0.67220400	0.00009700
	N10	3.56526000	−0.39981600	0.00040300
	H11	−1.91807500	1.96378500	0.00016800
	H12	1.91877100	1.67476400	−0.00053300
	H13	0.73147200	2.62963000	−0.89531300
	H14	0.73204600	2.62928600	0.89540500
	H15	−3.93391500	0.34219600	0.00043500
	H16	−3.52851500	−1.15391500	−0.89190000
	H17	−3.52824900	−1.15417100	0.89221900
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −484.9450554 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S48: Salt 48

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.67468300	0.00935200	−0.00001100
	N2	0.12778500	−1.06305900	0.00037200
	N3	1.46009600	−0.72163800	−0.00059300
	C4	1.46120000	0.56763800	0.00028800

	N5	0.16620400	1.07016600	−0.00002300
	N6	−2.00636100	0.03613400	−0.00011800
	H7	−0.13122800	−2.04067600	0.00063500
	H8	2.34086100	1.19145000	0.00034700
	H9	−0.09999700	2.04618100	0.00021400
	H10	−2.54623400	−0.81626400	0.00015500
	H11	−2.51656700	0.90615400	−0.00048200
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −298.0636709 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S49: Salt 49

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.72573800	−1.43573300	0.00000000
	C2	1.10022700	−0.18529000	0.00000000
	N3	0.00000000	0.65115400	0.00000000
	C4	−1.08228900	−0.13710400	0.00000000
	N5	−0.61573600	−1.38850300	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	2.12050200	0.16391300	0.00000000
	H8	−2.11338600	0.17676100	0.00000000
	H9	−1.15210300	−2.24869500	0.00000000
	H10	0.92340300	2.46433500	0.00000000

	H11	−0.84244300	2.51536000	0.00000000
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S50: Salt 50

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.47534100	−0.62785300	0.00003000
	N2	−1.47587000	0.62752200	−0.00006500
	N3	−0.17047500	1.05257900	0.00004300
	C4	0.66687500	0.00044000	0.00000300
	N5	−0.17063300	−1.05243600	−0.00001100
	N6	1.99178000	−0.00011800	−0.00001900
	H7	0.03292400	2.04532000	0.00005500
	H8	0.03343500	−2.04505300	0.00011200
	H9	2.51851900	0.86180900	0.00006500
	H10	2.51764600	−0.86257100	−0.00009200
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500

	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −314.0552154 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S51: Salt 51

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.64787200	1.13566200	−0.06142100
	C2	2.86433100	0.94984000	−0.63606800
	N3	3.16446100	−0.39148900	−0.49628800
	C4	2.17674400	−1.01703300	0.13675800
	N5	1.22537500	−0.10623900	0.41089400
	C6	0.00916300	−0.37648500	1.19147100
	N7	−1.22880200	−0.16276700	0.43452600
	C8	−1.83487400	−1.06326300	−0.36118800
	N9	−2.95332600	−0.50874200	−0.81761500
	C10	−3.09431100	0.76884800	−0.31097100
	C11	−2.01279400	0.99019700	0.48007900
	H12	1.06497600	2.03401400	0.05321800
	H13	3.53221200	1.64678700	−1.11641500
	H14	4.01885700	−0.83999300	−0.81505800
	H15	2.15645500	−2.06343700	0.39998000
	H16	0.04690200	−1.40701800	1.54124300
	H17	−0.01128500	0.28186300	2.05938100
	H18	−1.48966000	−2.06121100	−0.58203800
	H19	−3.61538100	−0.97269300	−1.43358900
	H20	−3.94084200	1.39511600	−0.54270700
	H21	−1.75297700	1.84464100	1.08340200
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300

	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −491.3068027 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S52: Salt 52

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.62853500	−1.19121100	−0.61498300
	C2	−2.82122300	−0.68378700	−1.02058800
	N3	−3.12051700	0.38479600	−0.19242000
	C4	−2.13842900	0.52984100	0.69082700
	N5	−1.20365400	−0.41489800	0.45708200
	C6	−0.01379400	−0.64351300	1.28615800
	N7	1.24769400	−0.43448400	0.57262000
	C8	1.89795200	0.73998100	0.43106700
	N9	3.03072800	0.52105500	−0.22763200
	C10	3.12680200	−0.82940700	−0.51866400
	C11	2.01764300	−1.43138600	−0.01746600
	C12	−4.34671100	1.20972000	−0.27251100
	C13	4.04645600	1.54044700	−0.57283500
	H14	−1.06502300	−2.02810800	−0.99183000
	H15	−3.47993600	−0.99520000	−1.81525500
	H16	−2.10666500	1.26737200	1.47735200
	H17	−0.06002500	0.02617800	2.14353100
	H18	−0.02476900	−1.67015700	1.65085200
	H19	1.56558900	1.69613000	0.80278800

	H20	3.97333600	−1.24466100	−1.04138600
	H21	1.72994000	−2.46995600	−0.00827900
	H22	−5.21426400	0.56913800	−0.11828700
	H23	−4.31095600	1.97227700	0.50258800
	H24	−4.39404600	1.68159900	−1.25310200
	H25	4.17199900	1.56363900	−1.65460100
	H26	3.70719600	2.51187000	−0.21968800
	H27	4.98690900	1.28047200	−0.08826000
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −569.967895 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S53: Salt 53

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.37381300	−1.31820500	−0.06154200
	C2	−2.53355700	−1.16897500	−0.63609400
	N3	−3.09988100	0.04683100	−0.31343000
	C4	−2.23229500	0.65978900	0.49349800
	N5	−1.19498500	−0.16706400	0.64411900
	C6	0.00005100	−0.00357900	1.46664200
	N7	1.19494100	0.16381000	0.64461500
	C8	2.23280800	−0.66175700	0.49088200
	N9	3.10004400	−0.04510800	−0.31361700

	C10	2.53293500	1.17154500	−0.63162300
	N11	1.37305900	1.31779300	−0.05655400
	C12	−4.41959000	0.55459300	−0.76432300
	C13	4.42006500	−0.55035400	−0.76643900
	H14	−3.00289400	−1.89933500	−1.27900000
	H15	−2.35011000	1.63604800	0.94005500
	H16	−0.12016200	0.88030000	2.09162300
	H17	0.12040900	−0.89048000	2.08729600
	H18	2.35127400	−1.63965400	0.93367400
	H19	3.00181000	1.90468800	−1.27169200
	H20	−4.42754800	0.59760800	−1.85251500
	H21	−5.19739500	−0.11587900	−0.40091200
	H22	−4.56886400	1.55081800	−0.35386600
	H23	4.42817900	−0.58885500	−1.85479700
	H24	5.19751100	0.11897200	−0.40015400
	H25	4.56973100	−1.54820200	−0.36009800
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −602.0167882 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S54: Salt 54

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.78681300	1.15357500	−0.00018800

	C2	2.14493400	1.26663800	−0.00005400
	N3	2.66044300	−0.01289200	0.00004400
	C4	1.63922300	−0.87746600	0.00001500
	N5	0.48930400	−0.19414000	−0.00013000
	C6	−4.54602400	0.43180200	0.00023600
	C7	−3.36875500	−0.54640400	−0.00002800
	C8	−2.01005100	0.17217000	0.00003700
	C9	−0.86201500	−0.83065100	−0.00025200
	C10	4.08826000	−0.37508200	0.00022500
	H11	0.02711100	1.91396500	−0.00030400
	H12	2.77586200	2.13896300	−0.00003800
	H13	1.72872000	−1.95159400	0.00008200
	H14	−5.49569200	−0.10660600	0.00017800
	H15	−4.52983400	1.07464300	0.88491500
	H16	−4.52993400	1.07499800	−0.88418700
	H17	−3.43357000	−1.19878700	−0.87800800
	H18	−3.43346700	−1.19914200	0.87769700
	H19	−1.94441900	0.81567700	0.88409700
	H20	−1.94454600	0.81605100	−0.88376000
	H21	−0.91103200	−1.46733700	−0.88607000
	H22	−0.91097100	−1.46776900	0.88525800
	H23	4.67311000	0.54169400	−0.00006200
	H24	4.32302700	−0.95121500	0.89461200
	H25	4.32309800	−0.95180700	−0.89376100
Anion	N1	0.66551300	3.68113200	0.00000000
	N2	−0.66551300	3.83151700	0.00000000
	N3	−1.24462900	2.63331700	0.00000000
	C4	−0.22031300	1.75474100	0.00000000
	N5	0.97206800	2.38478800	0.00000000
	C6	0.22031300	−1.75474100	0.00000000
	N7	1.24462900	−2.63331700	0.00000000
	N8	0.66551300	−3.83151700	0.00000000
	N9	−0.66551300	−3.68113200	0.00000000
	N10	−0.97206800	−2.38478800	0.00000000
	N11	−0.50128100	0.38137300	0.00000000
	N12	0.50128100	−0.38137300	0.00000000

SCF Done: E(B3LYP, cation) = −423.2848953 a.u.

SCF Done: E(B3LYP, anion) = −623.7876469 a.u.

Table S55: Salt 55

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.37645700	−0.26725600	0.00013500
	C2	0.72052100	−1.07657400	0.00015500
	N3	1.81260500	−0.24567800	0.00001000
	C4	1.38279000	1.02472300	−0.00013800
	N5	0.04834900	1.05155300	−0.00009100
	N6	−1.76672600	−0.69539800	0.00000400
	O7	−1.94271500	−1.89826000	−0.00027700
	O8	−2.61598000	0.18102900	0.00020900
	C9	−0.75882600	2.29636600	−0.00001800
	C10	3.22317100	−0.67991200	0.00003500
	H11	0.78492900	−2.15207200	0.00026700
	H12	2.01767400	1.89617200	−0.00032800
	H13	−1.38498700	2.32179800	−0.88835600
	H14	−1.38471900	2.32182800	0.88850400
	H15	−0.06349400	3.13332300	−0.00014200
	H16	3.41642000	−1.27071100	0.89449900
	H17	3.41618700	−1.27155400	−0.89392100
	H18	3.86075600	0.20164600	−0.00045100
Anion	N1	0.66551300	3.68113200	0.00000000
	N2	−0.66551300	3.83151700	0.00000000
	N3	−1.24462900	2.63331700	0.00000000
	C4	−0.22031300	1.75474100	0.00000000
	N5	0.97206800	2.38478800	0.00000000
	C6	0.22031300	−1.75474100	0.00000000
	N7	1.24462900	−2.63331700	0.00000000
	N8	0.66551300	−3.83151700	0.00000000
	N9	−0.66551300	−3.68113200	0.00000000
	N10	−0.97206800	−2.38478800	0.00000000
	N11	−0.50128100	0.38137300	0.00000000
	N12	0.50128100	−0.38137300	0.00000000

SCF Done: E(B3LYP, cation) = −509.839047 a.u.

SCF Done: E(B3LYP, anion) = −623.7876469 a.u.

Table S56: Salt 56

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.59451600	1.20187700	−0.00003200
	N2	0.70987100	1.21521700	−0.00001400
	N3	1.06725400	−0.09451300	0.00000000
	C4	0.00077400	−0.88021700	−0.00013000

	N5	−1.08025000	−0.08242400	−0.00002500
	C6	−2.49413600	−0.50489600	0.00008000
	C7	2.48650600	−0.47089700	0.00007100
	H8	−1.22032700	2.08055400	−0.00001100
	H9	−0.00234600	−1.95863900	−0.00020400
	H10	−3.11391800	0.38900000	0.00000800
	H11	−2.70184400	−1.08933900	−0.89524100
	H12	−2.70178700	−1.08916200	0.89553200
	H13	2.55902600	−1.55669300	0.00020400
	H14	2.95566400	−0.05954800	−0.89231300
	H15	2.95564100	−0.05933200	0.89236600
Anion	N1	0.66551300	3.68113200	0.00000000
	N2	−0.66551300	3.83151700	0.00000000
	N3	−1.24462900	2.63331700	0.00000000
	C4	−0.22031300	1.75474100	0.00000000
	N5	0.97206800	2.38478800	0.00000000
	C6	0.22031300	−1.75474100	0.00000000
	N7	1.24462900	−2.63331700	0.00000000
	N8	0.66551300	−3.83151700	0.00000000
	N9	−0.66551300	−3.68113200	0.00000000
	N10	−0.97206800	−2.38478800	0.00000000
	N11	−0.50128100	0.38137300	0.00000000
	N12	0.50128100	−0.38137300	0.00000000

SCF Done: E(B3LYP, cation) = −321.329351 a.u.

SCF Done: E(B3LYP, anion) = −623.7876469 a.u.

Table S57: Salt 57

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.18477700	−0.48806600	−0.00017100
	N2	−0.95937800	−1.14105000	−0.00018500
	N3	−1.91196800	−0.18023500	0.00005300
	C4	−1.38445400	1.02649200	0.00005300
	N5	−0.04134400	0.88642500	−0.00005800
	C6	0.89524300	2.03075200	−0.00012200
	C7	−3.32873300	−0.56230300	0.00021500
	N8	1.34903900	−1.20352600	−0.00035600
	N9	2.47345600	−0.67220400	0.00009700
	N10	3.56526000	−0.39981600	0.00040300
	H11	−1.91807500	1.96378500	0.00016800
	H12	1.91877100	1.67476400	−0.00053300

	H13	0.73147200	2.62963000	−0.89531300
	H14	0.73204600	2.62928600	0.89540500
	H15	−3.93391500	0.34219600	0.00043500
	H16	−3.52851500	−1.15391500	−0.89190000
	H17	−3.52824900	−1.15417100	0.89221900
Anion	N1	0.66551300	3.68113200	0.00000000
	N2	−0.66551300	3.83151700	0.00000000
	N3	−1.24462900	2.63331700	0.00000000
	C4	−0.22031300	1.75474100	0.00000000
	N5	0.97206800	2.38478800	0.00000000
	C6	0.22031300	−1.75474100	0.00000000
	N7	1.24462900	−2.63331700	0.00000000
	N8	0.66551300	−3.83151700	0.00000000
	N9	−0.66551300	−3.68113200	0.00000000
	N10	−0.97206800	−2.38478800	0.00000000
	N11	−0.50128100	0.38137300	0.00000000
	N12	0.50128100	−0.38137300	0.00000000

SCF Done: E(B3LYP, cation) = −484.9450554 a.u.

SCF Done: E(B3LYP, anion) = −623.7876469 a.u.

Table S58: Salt 58

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.67062800	1.21160500	0.00003500
	C2	0.63691100	1.18917700	−0.00001800
	N3	1.09525400	−0.10727600	−0.00002800
	C4	0.00744600	−0.89435100	0.00000600
	N5	−1.04914100	−0.07890200	0.00001700
	N6	2.39810400	−0.50640700	−0.00006700
	C7	−2.47273800	−0.43828300	0.00006100
	H8	1.27858000	2.05575300	−0.00003600
	H9	−0.00304800	−1.97160800	0.00000600
	H10	3.10846400	0.20392000	−0.00009900
	H11	2.60559400	−1.48918100	−0.00007600
	H12	−2.55730100	−1.52323800	−0.00009900
	H13	−2.93850600	−0.02415500	0.89301100
	H14	−2.93861800	−0.02388600	−0.89270400
Anion	N1	0.66551300	3.68113200	0.00000000
	N2	−0.66551300	3.83151700	0.00000000
	N3	−1.24462900	2.63331700	0.00000000
	C4	−0.22031300	1.75474100	0.00000000

	N5	0.97206800	2.38478800	0.00000000
	C6	0.22031300	−1.75474100	0.00000000
	N7	1.24462900	−2.63331700	0.00000000
	N8	0.66551300	−3.83151700	0.00000000
	N9	−0.66551300	−3.68113200	0.00000000
	N10	−0.97206800	−2.38478800	0.00000000
	N11	−0.50128100	0.38137300	0.00000000
	N12	0.50128100	−0.38137300	0.00000000

SCF Done: E(B3LYP, cation) = −337.3261717 a.u.

SCF Done: E(B3LYP, anion) = −623.7876469 a.u.

Table S59: Salt 59

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	0.59401000	1.20341000	−0.00008700
	N2	−0.70712400	1.21582900	0.00017200
	N3	−1.06118300	−0.10562400	0.00022600
	C4	−0.00316900	−0.90017700	−0.00023200
	N5	1.07066800	−0.09532700	−0.00063300
	N6	2.38079800	−0.58790700	0.00029200
	N7	−2.37221900	−0.56044600	0.00014800
	H8	1.22888500	2.07678200	−0.00042500
	H9	0.00090700	−1.97858500	−0.00050200
	H10	2.86658100	−0.28191500	0.83865900
	H11	2.86833300	−0.28067400	−0.83657800
	H12	−2.84360300	−0.20986000	0.83125400
	H13	−2.84272500	−0.21082700	−0.83192800
Anion	N1	0.66551300	3.68113200	0.00000000
	N2	−0.66551300	3.83151700	0.00000000
	N3	−1.24462900	2.63331700	0.00000000
	C4	−0.22031300	1.75474100	0.00000000
	N5	0.97206800	2.38478800	0.00000000
	C6	0.22031300	−1.75474100	0.00000000
	N7	1.24462900	−2.63331700	0.00000000
	N8	0.66551300	−3.83151700	0.00000000
	N9	−0.66551300	−3.68113200	0.00000000
	N10	−0.97206800	−2.38478800	0.00000000
	N11	−0.50128100	0.38137300	0.00000000
	N12	0.50128100	−0.38137300	0.00000000

SCF Done: E(B3LYP, cation) = −353.3536473 a.u.

SCF Done: E(B3LYP, anion) = −623.7876469 a.u.

Table S60: Salt 60

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.63151800	−1.53175700	0.00017900
	N2	−0.63750600	−1.53002600	−0.00069800
	N3	−1.05571500	−0.23777700	0.00005900
	C4	0.00062000	0.58293300	−0.00017600
	N5	1.05612100	−0.24001700	0.00002300
	C6	2.49454500	0.06414800	0.00026300
	C7	0.00297500	2.06623300	−0.00026200
	C8	−2.49346800	0.06453600	0.00041600
	H9	3.01255800	−0.89198200	0.00052200
	H10	2.75264700	0.62484100	−0.89737600
	H11	2.75226100	0.62510600	0.89784600
	H12	1.02206200	2.44947700	−0.00006000
	H13	−0.50977200	2.44820700	−0.88677800
	H14	−0.51016600	2.44831600	0.88597600
	H15	−2.62545000	1.14379800	0.00106400
	H16	−2.94165000	−0.36839200	−0.89268300
	H17	−2.94145100	−0.36943600	0.89310700
Anion	N1	0.66551300	3.68113200	0.00000000
	N2	−0.66551300	3.83151700	0.00000000
	N3	−1.24462900	2.63331700	0.00000000
	C4	−0.22031300	1.75474100	0.00000000
	N5	0.97206800	2.38478800	0.00000000
	C6	0.22031300	−1.75474100	0.00000000
	N7	1.24462900	−2.63331700	0.00000000
	N8	0.66551300	−3.83151700	0.00000000
	N9	−0.66551300	−3.68113200	0.00000000
	N10	−0.97206800	−2.38478800	0.00000000
	N11	−0.50128100	0.38137300	0.00000000
	N12	0.50128100	−0.38137300	0.00000000

SCF Done: E(B3LYP, cation) = −376.6673328 a.u.

SCF Done: E(B3LYP, anion) = −623.7876469 a.u.

Table S61: Salt 61

Cartesian coordinates

	Atom	X	Y	Z

Cation	N1	0.72573800	−1.43573300	0.00000000
	C2	1.10022700	−0.18529000	0.00000000
	N3	0.00000000	0.65115400	0.00000000
	C4	−1.08228900	−0.13710400	0.00000000
	N5	−0.61573600	−1.38850300	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	2.12050200	0.16391300	0.00000000
	H8	−2.11338600	0.17676100	0.00000000
	H9	−1.15210300	−2.24869500	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000
Anion	N1	0.00000000	−3.01602700	−0.99279100
	N2	0.00000000	−3.41216300	0.25817100
	N3	0.00000000	−2.33510900	1.07581300
	C4	0.00000000	−1.28379000	0.23118600
	N5	0.00000000	−1.65522400	−1.05079800
	C6	0.00000000	1.28379000	0.23118600
	N7	0.00000000	2.33510900	1.07581300
	N8	0.00000000	3.41216300	0.25817100
	N9	0.00000000	3.01602700	−0.99279100
	N10	0.00000000	1.65522400	−1.05079800
	N11	0.00000000	0.00000000	0.76918300
	H12	0.00000000	0.00000000	1.77595000

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −569.6559441 a.u.

Table S62: Salt 62

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.72573800	−1.43573300	0.00000000
	C2	1.10022700	−0.18529000	0.00000000
	N3	0.00000000	0.65115400	0.00000000
	C4	−1.08228900	−0.13710400	0.00000000
	N5	−0.61573600	−1.38850300	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	2.12050200	0.16391300	0.00000000
	H8	−2.11338600	0.17676100	0.00000000
	H9	−1.15210300	−2.24869500	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000
Anion	N1	−0.36965900	2.81889800	0.00000000

	N2	0.94888300	2.68000500	0.00000000
	N3	1.26302000	1.37463600	0.00000000
	C4	0.07711200	0.73207500	0.00000000
	N5	−0.94888300	1.60762500	0.00000000
	C6	−0.07711200	−0.73207500	0.00000000
	N7	−1.26302000	−1.37463600	0.00000000
	N8	−0.94888300	−2.68000500	0.00000000
	N9	0.36965900	−2.81889800	0.00000000
	N10	0.94888300	−1.60762500	0.00000000

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −514.2825578 a.u.

Table S63: Salt 63

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−2.30865200	0.81588100	0.00000000
	C2	−1.21694900	0.03718400	0.00000000
	N3	0.00000000	0.64962600	0.00000000
	N4	−1.29726400	−1.27578000	0.00000000
	C5	1.27171000	0.00451000	0.00000000
	N6	2.30605800	0.88525700	0.00000000
	N7	1.30701300	−1.27093700	0.00000000
	H8	−3.23217400	0.41098700	0.00000000
	H9	−2.25308100	1.82198600	0.00000000
	H10	−0.00498400	1.65842700	0.00000000
	H11	−0.38525300	−1.77463900	0.00000000
	H12	−2.18726700	−1.75083000	0.00000000
	H13	3.25154100	0.53751900	0.00000000
	H14	2.19157500	1.88552200	0.00000000
	H15	2.24099900	−1.66747000	0.00000000
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −354.7051979 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S64: Salt 64

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.72573800	−1.43573300	0.00000000
	C2	1.10022700	−0.18529000	0.00000000
	N3	0.00000000	0.65115400	0.00000000
	C4	−1.08228900	−0.13710400	0.00000000
	N5	−0.61573600	−1.38850300	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	2.12050200	0.16391300	0.00000000
	H8	−2.11338600	0.17676100	0.00000000
	H9	−1.15210300	−2.24869500	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S65: Salt 65

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800
	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200
	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	N1	−0.65342100	−1.43332300	0.00000000

	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S66: Salt 66

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.71309600	1.63579100	0.00000000
	C2	0.00000000	0.49075400	0.00000000
	N3	1.34087600	0.55400700	0.00000000
	N4	−0.63397000	−0.66964200	0.00000000
	N5	−0.05044100	−1.92877000	0.00000000
	H6	−1.72036800	1.63935700	0.00000000
	H7	−0.25478500	2.53240900	0.00000000
	H8	1.92947100	−0.26070500	0.00000000
	H9	1.81369600	1.44397200	0.00000000
	H10	−1.64306300	−0.68139000	0.00000000
	H11	−0.67178300	−2.71571000	0.00000000
	H12	0.94325200	−2.04216900	0.00000000
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S67: Salt 67

Cartesian coordinates

	Atom	X	Y	Z

Cation	N1	−0.67062800	1.21160500	0.00003500
	C2	0.63691100	1.18917700	−0.00001800
	N3	1.09525400	−0.10727600	−0.00002800
	C4	0.00744600	−0.89435100	0.00000600
	N5	−1.04914100	−0.07890200	0.00001700
	N6	2.39810400	−0.50640700	−0.00006700
	C7	−2.47273800	−0.43828300	0.00006100
	H8	1.27858000	2.05575300	−0.00003600
	H9	−0.00304800	−1.97160800	0.00000600
	H10	3.10846400	0.20392000	−0.00009900
	H11	2.60559400	−1.48918100	−0.00007600
	H12	−2.55730100	−1.52323800	−0.00009900
	H13	−2.93850600	−0.02415500	0.89301100
	H14	−2.93861800	−0.02388600	−0.89270400
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −337.3261717 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S68: Salt68

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.59982300	0.37475000	0.00003300
	C2	0.18818000	−0.70188400	−0.00004000
	N3	1.45301300	−0.24863300	−0.00002100
	C4	1.37531000	1.12268300	0.00005700
	N5	0.12574600	1.50822600	0.00006800
	C6	−2.08310200	0.45012700	0.00007500
	C7	−2.74410400	−0.91760400	−0.00006600
	N8	2.59284000	−0.99779000	−0.00007200
	H9	−0.11646900	−1.73397100	−0.00009600
	H10	2.23286600	1.77632500	0.00008500
	H11	−2.35238200	1.03043200	0.88364600
	H12	−2.35241300	1.03062900	−0.88335700
	H13	−3.82529800	−0.77126500	−0.00003900

	H14	−2.49786600	−1.49687700	−0.89341700
	H15	−2.49785300	−1.49706900	0.89315700
	H16	3.47355600	−0.51498900	−0.00005400
	H17	2.51572000	−1.99902500	−0.00013900
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −376.655599 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S69: Salt 69

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.63269500	−1.51124800	−0.00011300
	N2	0.62505200	−1.53675300	−0.00001300
	N3	1.07010900	−0.23384900	0.00000600
	C4	0.01446400	0.60794500	−0.00009200
	N5	−1.05586200	−0.19902300	−0.00023900
	C6	−2.48172900	0.13532800	0.00023400
	N7	0.08185300	1.93048400	−0.00009700
	N8	2.38626800	0.17796600	0.00015600
	H9	−3.02338200	−0.80823600	−0.00003000
	H10	−2.73269300	0.69853500	0.90000200
	H11	−2.73312300	0.69925100	−0.89896200
	H12	0.99472500	2.36812900	0.00001100
	H13	−0.74240900	2.51138700	−0.00015600
	H14	2.85860500	−0.16092000	0.83499900
	H15	2.85878700	−0.16083300	−0.83461900
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −408.7379057 a.u.
SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S70: Salt 70

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.60584700	−1.52255200	0.00008900
	N2	−0.65427800	−1.50393700	−0.00028300
	N3	−1.07049400	−0.19824200	0.00003200
	C4	0.00675400	0.60547600	−0.00006000
	N5	1.06035500	−0.23187400	−0.00001500
	C6	2.49252300	0.07273700	0.00010900
	N7	0.04688700	1.93796900	−0.00011200
	C8	−2.50303000	0.11401600	0.00015500
	H9	3.01461000	−0.88165800	0.00024300
	H10	2.75697800	0.63012500	−0.89975200
	H11	2.75677200	0.63026100	0.89994600
	H12	−0.79576700	2.49123100	−0.00002800
	H13	0.92630800	2.43182100	−0.00019300
	H14	−2.63741500	1.19426500	0.00067300
	H15	−2.95858400	−0.30906800	−0.89398900
	H16	−2.95859700	−0.30990500	0.89389500
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −392.7171077 a.u.
SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S71: Salt 71

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	1.27417300	−0.01552500	0.00000500
	N2	0.55269800	−1.08300800	−0.00002100
	N3	−0.69851400	−0.61966400	−0.00000600

	C4	−0.66889800	0.74822700	0.00000100
	N5	0.60502600	1.13911600	−0.00009800
	C6	2.74552400	−0.06569500	0.00004900
	N7	−1.73412800	1.55395200	0.00002100
	C8	−1.84749600	−1.53064500	−0.00000200
	H9	3.09281800	0.96331900	−0.00039000
	H10	3.07745200	−0.58854200	0.89545800
	H11	3.07745600	−0.58931300	−0.89490600
	H12	−2.67778700	1.20353900	0.00023000
	H13	−1.59277400	2.55314800	0.00003200
	H14	−1.45920400	−2.54619500	−0.00015600
	H15	−2.44368800	−1.36579600	0.89843700
	H16	−2.44384400	−1.36558900	−0.89829900
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000
	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −392.7214667 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S72: Salt 72

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.42331100	0.37619100	0.00000900
	N2	−1.53125400	−0.98612800	−0.00000800
	N3	−0.36799900	−1.46344200	0.00003100
	N4	0.53644700	−0.42712400	−0.00002100
	C5	−0.12717000	0.74116100	−0.00000700
	N6	0.36787200	1.97495300	0.00001600
	C7	1.97512400	−0.71509900	−0.00000300
	H8	−2.25955300	0.94762800	−0.00012500
	H9	1.36252400	2.14220400	−0.00004700
	H10	−0.23662100	2.78319300	0.00006300
	H11	2.53118400	0.22069200	−0.00040200
	H12	2.22129800	−1.28529400	0.89448400
	H13	2.22115600	−1.28594600	−0.89411100
Anion	C1	0.58282500	−1.22389200	−0.00000300

	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −353.3859539 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S73: Salt 73

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.08662300	−0.15534200	−0.00000800
	N2	−0.65252700	1.14258300	0.00002400
	N3	0.68150600	1.18024000	−0.00004600
	N4	1.00507800	−0.06381800	−0.00003300
	N5	−0.00612000	−0.93627200	−0.00010500
	C6	2.40732000	−0.50516200	0.00006900
	N7	−2.35101200	−0.57034900	0.00006500
	H8	−1.16666800	2.01634000	0.00002000
	H9	3.03008400	0.38546200	−0.00005900
	H10	2.57322900	−1.10420700	0.89413500
	H11	2.57324900	−1.10448700	−0.89380500
	H12	−3.13260900	0.06557500	0.00003500
	H13	−2.53993900	−1.56234600	−0.00002400
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500

	C6	1.41054200	0.01531000	−0.00003500
	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −353.391606 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S74: Salt 74

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.60584700	−1.52255200	0.00008900
	N2	−0.65427800	−1.50393700	−0.00028300
	N3	−1.07049400	−0.19824200	0.00003200
	C4	0.00675400	0.60547600	−0.00006000
	N5	1.06035500	−0.23187400	−0.00001500
	C6	2.49252300	0.07273700	0.00010900
	N7	0.04688700	1.93796900	−0.00011200
	C8	−2.50303000	0.11401600	0.00015500
	H9	3.01461000	−0.88165800	0.00024300
	H10	2.75697800	0.63012500	−0.89975200
	H11	2.75677200	0.63026100	0.89994600
	H12	−0.79576700	2.49123100	−0.00002800
	H13	0.92630800	2.43182100	−0.00019300
	H14	−2.63741500	1.19426500	0.00067300
	H15	−2.95858400	−0.30906800	−0.89398900
	H16	−2.95859700	−0.30990500	0.89389500
Anion	C1	0.58282500	−1.22389200	−0.00000300
	C2	−0.79148400	−1.22195000	0.00001300
	C3	−1.49693900	−0.01630200	0.00001200
	C4	−0.81787400	1.20442100	0.00000600
	C5	0.55605200	1.23619400	−0.00000500
	C6	1.41054200	0.01531000	−0.00003500

	O7	2.63157300	0.02862800	−0.00015200
	N8	1.21373900	−2.54756700	0.00000400
	O9	2.43431100	−2.63285700	0.00013200
	O10	0.46971900	−3.54039400	−0.00014400
	N11	1.15804600	2.57326400	0.00000800
	O12	2.37646400	2.68515000	0.00031400
	O13	0.39260200	3.54965800	−0.00026500
	N14	−2.93812400	−0.03188200	0.00003700
	O15	−3.53876700	1.04886800	0.00003400
	O16	−3.51537200	−1.12530600	0.00004200
	H17	−1.32596500	−2.16021500	0.00002700
	H18	−1.37263400	2.13084200	0.00001500

SCF Done: E(B3LYP, cation) = −392.7171077 a.u.

SCF Done: E(B3LYP, anion) = −920.7359569 a.u.

Table S75: Salt 75

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.60584700	−1.52255200	0.00008900
	N2	−0.65427800	−1.50393700	−0.00028300
	N3	−1.07049400	−0.19824200	0.00003200
	C4	0.00675400	0.60547600	−0.00006000
	N5	1.06035500	−0.23187400	−0.00001500
	C6	2.49252300	0.07273700	0.00010900
	N7	0.04688700	1.93796900	−0.00011200
	C8	−2.50303000	0.11401600	0.00015500
	H9	3.01461000	−0.88165800	0.00024300
	H10	2.75697800	0.63012500	−0.89975200
	H11	2.75677200	0.63026100	0.89994600
	H12	−0.79576700	2.49123100	−0.00002800
	H13	0.92630800	2.43182100	−0.00019300
	H14	−2.63741500	1.19426500	0.00067300
	H15	−2.95858400	−0.30906800	−0.89398900
	H16	−2.95859700	−0.30990500	0.89389500
Anion	N1	−0.65342100	−1.43332300	0.00000000
	N2	0.65342800	−1.43330900	0.00000000
	N3	1.11552800	−0.15197500	0.00000000
	C4	0.00000000	0.57947300	0.00000000
	N5	−1.11552100	−0.15199200	0.00000000
	N6	−0.00001000	1.96951600	0.00000000
	H7	0.87011600	2.46537900	0.00000000

	H8	−0.87014500	2.46536400	0.00000000

SCF Done: E(B3LYP, cation) = −392.7171077 a.u.

SCF Done: E(B3LYP, anion) = −313.1609514 a.u.

Table S76: Salt 76

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.42331100	0.37619100	0.00000900
	N2	−1.53125400	−0.98612800	−0.00000800
	N3	−0.36799900	−1.46344200	0.00003100
	N4	0.53644700	−0.42712400	−0.00002100
	C5	−0.12717000	0.74116100	−0.00000700
	N6	0.36787200	1.97495300	0.00001600
	C7	1.97512400	−0.71509900	−0.00000300
	H8	−2.25955300	0.94762800	−0.00012500
	H9	1.36252400	2.14220400	−0.00004700
	H10	−0.23662100	2.78319300	0.00006300
	H11	2.53118400	0.22069200	−0.00040200
	H12	2.22129800	−1.28529400	0.89448400
	H13	2.22115600	−1.28594600	−0.89411100
Anion	N1	−2.32247300	0.87855400	−0.00183500
	N2	−2.67204900	−0.36336800	0.00118900
	N3	−1.51240300	−1.05963800	0.00193100
	C4	−0.44794900	−0.20055100	−0.00041000
	N5	−0.97156800	1.03677900	−0.00288600
	N6	0.77606400	−0.78173600	−0.00100400
	N7	1.86650100	0.00782200	0.00028500
	O8	2.96076700	−0.59346500	−0.00249500
	O9	1.79276000	1.24847900	0.00420900
	H10	−1.48903200	−2.06571300	0.00499100

SCF Done: E(B3LYP, cation) = −353.3859539 a.u.

SCF Done: E(B3LYP, anion) = −517.7219762 a.u.

Table S77: Salt 77

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.72573800	−1.43573300	0.00000000
	C2	1.10022700	−0.18529000	0.00000000
	N3	0.00000000	0.65115400	0.00000000

	C4	−1.08228900	−0.13710400	0.00000000
	N5	−0.61573600	−1.38850300	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	2.12050200	0.16391300	0.00000000
	H8	−2.11338600	0.17676100	0.00000000
	H9	−1.15210300	−2.24869500	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000
Anion	N1	−2.32247300	0.87855400	−0.00183500
	N2	−2.67204900	−0.36336800	0.00118900
	N3	−1.51240300	−1.05963800	0.00193100
	C4	−0.44794900	−0.20055100	−0.00041000
	N5	−0.97156800	1.03677900	−0.00288600
	N6	0.77606400	−0.78173600	−0.00100400
	N7	1.86650100	0.00782200	0.00028500
	O8	2.96076700	−0.59346500	−0.00249500
	O9	1.79276000	1.24847900	0.00420900
	H10	−1.48903200	−2.06571300	0.00499100

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −517.7219762 a.u.

Table S78: Salt 78

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.47534100	−0.62785300	0.00003000
	N2	−1.47587000	0.62752200	−0.00006500
	N3	−0.17047500	1.05257900	0.00004300
	C4	0.66687500	0.00044000	0.00000300
	N5	−0.17063300	−1.05243600	−0.00001100
	N6	1.99178000	−0.00011800	−0.00001900
	H7	0.03292400	2.04532000	0.00005500
	H8	0.03343500	−2.04505300	0.00011200
	H9	2.51851900	0.86180900	0.00006500
	H10	2.51764600	−0.86257100	−0.00009200
Anion	N1	−2.32247300	0.87855400	−0.00183500
	N2	−2.67204900	−0.36336800	0.00118900
	N3	−1.51240300	−1.05963800	0.00193100
	C4	−0.44794900	−0.20055100	−0.00041000
	N5	−0.97156800	1.03677900	−0.00288600
	N6	0.77606400	−0.78173600	−0.00100400
	N7	1.86650100	0.00782200	0.00028500

	O8	2.96076700	−0.59346500	−0.00249500
	O9	1.79276000	1.24847900	0.00420900
	H10	−1.48903200	−2.06571300	0.00499100

SCF Done: E(B3LYP, cation) = −314.0552154 a.u.

SCF Done: E(B3LYP, anion) = −517.7219762 a.u.

Table S79: Salt 79

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.06640500	−0.41832800	−0.00003200
	N2	0.03611200	−1.21412900	−0.00000400
	N3	−1.03285300	−0.37700300	0.00003700
	C4	−0.67974900	0.89734900	−0.00005800
	N5	0.65865300	0.89769800	0.00002500
	H6	2.09788600	−0.73449200	−0.00004900
	H7	−1.97156900	−0.76356700	0.00008100
	H8	−1.33192900	1.75728600	−0.00010100
	H9	1.25228900	1.72069000	0.00019900
Anion	N1	−2.32247300	0.87855400	−0.00183500
	N2	−2.67204900	−0.36336800	0.00118900
	N3	−1.51240300	−1.05963800	0.00193100
	C4	−0.44794900	−0.20055100	−0.00041000
	N5	−0.97156800	1.03677900	−0.00288600
	N6	0.77606400	−0.78173600	−0.00100400
	N7	1.86650100	0.00782200	0.00028500
	O8	2.96076700	−0.59346500	−0.00249500
	O9	1.79276000	1.24847900	0.00420900
	H10	−1.48903200	−2.06571300	0.00499100

SCF Done: E(B3LYP, cation) = −242.6694066 a.u.

SCF Done: E(B3LYP, anion) = −517.7219762 a.u.

Table S80: Salt 80

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	1.40163300	−1.16761600	−0.00007100
	C2	2.51483200	−0.49231500	0.00013100
	N3	2.25644600	0.85524600	0.00007900
	C4	0.91889400	0.99427800	−0.00020700
	N5	0.41456800	−0.22667700	−0.00007100

	C6	−3.43539600	−0.01830700	0.00007700
	C7	−1.99159400	0.49998300	0.00007900
	C8	−1.00583700	−0.66235400	−0.00008000
	H9	3.50410500	−0.92217700	0.00027700
	H10	2.93320700	1.60949100	0.00033100
	H11	0.37374200	1.92323300	−0.00035800
	H12	−4.13480900	0.81855200	0.00017800
	H13	−3.64096400	−0.62465800	−0.88531000
	H14	−3.64090600	−0.62482500	0.88536300
	H5	−1.83161800	1.12538300	0.88534200
	H16	−1.83169100	1.12557000	−0.88506600
	H17	−1.12251300	−1.29236900	−0.88378500
	H18	−1.12247600	−1.29258600	0.88347700
Anion	N1	−2.32247300	0.87855400	−0.00183500
	N2	−2.67204900	−0.36336800	0.00118900
	N3	−1.51240300	−1.05963800	0.00193100
	C4	−0.44794900	−0.20055100	−0.00041000
	N5	−0.97156800	1.03677900	−0.00288600
	N6	0.77606400	−0.78173600	−0.00100400
	N7	1.86650100	0.00782200	0.00028500
	O8	2.96076700	−0.59346500	−0.00249500
	O9	1.79276000	1.24847900	0.00420900
	H10	−1.48903200	−2.06571300	0.00499100

SCF Done: E(B3LYP, cation) = −360.6577174 a.u.

SCF Done: E(B3LYP, anion) = −517.7219762 a.u.

Table S81: Salt 81

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	1.16549400	−1.15216600	−0.00009000
	C2	0.10928300	−0.37050500	−0.00001000
	N3	0.50786700	0.96531600	0.00002000
	C4	1.85243700	0.97271400	−0.00003500
	N5	2.21450300	−0.29340200	0.00006400
	N6	−1.15653700	−0.87371600	0.00003400
	N7	−2.11886300	−0.07468100	0.00000600
	N8	−3.09035500	0.48886000	0.00000100
	H9	−0.07760900	1.79315200	−0.00011500
	H10	2.49471700	1.83993100	−0.00001900
	H11	3.15781300	−0.66781200	0.00015800
Anion	N1	−2.32247300	0.87855400	−0.00183500

	N2	−2.67204900	−0.36336800	0.00118900
	N3	−1.51240300	−1.05963800	0.00193100
	C4	−0.44794900	−0.20055100	−0.00041000
	N5	−0.97156800	1.03677900	−0.00288600
	N6	0.77606400	−0.78173600	−0.00100400
	N7	1.86650100	0.00782200	0.00028500
	O8	2.96076700	−0.59346500	−0.00249500
	O9	1.79276000	1.24847900	0.00420900
	H10	−1.48903200	−2.06571300	0.00499100

SCF Done: E(B3LYP, cation) = −406.2900901 a.u.

SCF Done: E(B3LYP, anion) = −517.7219762 a.u.

Table S82: Salt 82

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800
	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200
	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	N1	1.90351300	−1.54547200	−0.00199900
	N2	2.47467700	−0.38740100	0.00007700
	N3	1.47137600	0.52258100	0.00055500
	C4	0.26720600	−0.13807500	−0.00127600
	N5	0.55138700	−1.45154400	−0.00282800
	N6	−0.84142100	0.64269300	−0.00277100
	C7	1.72226000	1.94519700	0.00298900
	N8	−2.05277700	0.05897300	0.00028300
	O9	−3.02371300	0.84619000	−0.00418400
	O10	−2.20279300	−1.17448400	0.00740700
	H11	0.75268400	2.44088200	0.00194300
	H12	2.28606900	2.23075300	0.89503200
	H13	2.28921300	2.23318000	−0.88626600

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −557.0437665 a.u.

Table S83: Salt 83

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.71309600	1.63579100	0.00000000
	C2	0.00000000	0.49075400	0.00000000
	N3	1.34087600	0.55400700	0.00000000
	N4	−0.63397000	−0.66964200	0.00000000
	N5	−0.05044100	−1.92877000	0.00000000
	H6	−1.72036800	1.63935700	0.00000000
	H7	−0.25478500	2.53240900	0.00000000
	H8	1.92947100	−0.26070500	0.00000000
	H9	1.81369600	1.44397200	0.00000000
	H10	−1.64306300	−0.68139000	0.00000000
	H11	−0.67178300	−2.71571000	0.00000000
	H12	0.94325200	−2.04216900	0.00000000
Anion	N1	1.90351300	−1.54547200	−0.00199900
	N2	2.47467700	−0.38740100	0.00007700
	N3	1.47137600	0.52258100	0.00055500
	C4	0.26720600	−0.13807500	−0.00127600
	N5	0.55138700	−1.45154400	−0.00282800
	N6	−0.84142100	0.64269300	−0.00277100
	C7	1.72226000	1.94519700	0.00298900
	N8	−2.05277700	0.05897300	0.00028300
	O9	−3.02371300	0.84619000	−0.00418400
	O10	−2.20279300	−1.17448400	0.00740700
	H11	0.75268400	2.44088200	0.00194300
	H12	2.28606900	2.23075300	0.89503200
	H13	2.28921300	2.23318000	−0.88626600

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −557.0437665 a.u.

Table S84: Salt 84

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.00000000	2.42944600	−0.09893800
	N2	0.00000000	1.14998700	−0.65450900
	C3	0.00000000	0.00000000	0.02528500
	N4	0.00000000	−1.14998700	−0.65450900
	N5	0.00000000	−2.42944600	−0.09893800

	N6	0.00000000	0.00000000	1.37233500
	H7	0.00000000	3.19851000	−0.74127800
	H8	0.00000000	2.56996300	0.89042200
	H9	0.00000000	1.13876300	−1.66204000
	H10	0.00000000	−1.13876300	−1.66204000
	H11	0.00000000	−3.19851000	−0.74127800
	H12	0.00000000	−2.56996300	0.89042200
	H13	0.00000000	−0.84963300	1.90800300
	H14	0.00000000	0.84963300	1.90800300
Anion	N1	1.90351300	−1.54547200	−0.00199900
	N2	2.47467700	−0.38740100	0.00007700
	N3	1.47137600	0.52258100	0.00055500
	C4	0.26720600	−0.13807500	−0.00127600
	N5	0.55138700	−1.45154400	−0.00282800
	N6	−0.84142100	0.64269300	−0.00277100
	C7	1.72226000	1.94519700	0.00298900
	N8	−2.05277700	0.05897300	0.00028300
	O9	−3.02371300	0.84619000	−0.00418400
	O10	−2.20279300	−1.17448400	0.00740700
	H11	0.75268400	2.44088200	0.00194300
	H12	2.28606900	2.23075300	0.89503200
	H13	2.28921300	2.23318000	−0.88626600

SCF Done: E(B3LYP, cation) = −316.4385003 a.u.

SCF Done: E(B3LYP, anion) = −557.0437665 a.u.

Table S85: Salt 85

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.73090600	1.42465800	0.00000000
	C2	0.00000000	0.28737400	0.00000000
	N3	1.33364100	0.45849100	0.00000000
	N4	−0.65902100	−0.87579600	0.00000000
	N5	2.38734200	−0.46354400	0.00000000
	N6	−0.19531500	−2.19352200	0.00000000
	N7	−2.12655000	1.51794100	0.00000000
	H8	−0.26473700	2.31587700	0.00000000
	H9	1.66735400	1.40846300	0.00000000
	H10	−1.66209300	−0.83875500	0.00000000
	H11	3.30922600	−0.07173500	0.00000000
	H12	2.24095500	−1.44742300	0.00000000
	H13	−0.89921200	−2.90635300	0.00000000

	H14	0.77363900	−2.41899000	0.00000000
	H15	−2.51076700	2.44330700	0.00000000
	H16	−2.71870400	0.71376600	0.00000000
Anion	N1	1.90351300	−1.54547200	−0.00199900
	N2	2.47467700	−0.38740100	0.00007700
	N3	1.47137600	0.52258100	0.00055500
	C4	0.26720600	−0.13807500	−0.00127600
	N5	0.55138700	−1.45154400	−0.00282800
	N6	−0.84142100	0.64269300	−0.00277100
	C7	1.72226000	1.94519700	0.00298900
	N8	−2.05277700	0.05897300	0.00028300
	O9	−3.02371300	0.84619000	−0.00418400
	O10	−2.20279300	−1.17448400	0.00740700
	H11	0.75268400	2.44088200	0.00194300
	H12	2.28606900	2.23075300	0.89503200
	H13	2.28921300	2.23318000	−0.88626600

SCF Done: E(B3LYP, cation) = −371.7391764 a.u.

SCF Done: E(B3LYP, anion) = −557.0437665 a.u.

Table S86: Salt 86

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.68202200	1.93302800	0.00000000
	C2	0.00000000	0.79762100	0.00000000
	N3	1.33107100	0.77740900	0.00000000
	N4	−0.78337800	−0.32289900	0.00000000
	N5	−0.22337400	−1.44878300	0.00000000
	N6	0.10039400	−2.52020000	0.00000000
	H7	−1.69293200	1.89950700	0.00000000
	H8	−0.23394500	2.83769500	0.00000000
	H9	1.85682500	−0.08467500	0.00000000
	H10	1.87121500	1.63185600	0.00000000
Anion	N1	1.90351300	−1.54547200	−0.00199900
	N2	2.47467700	−0.38740100	0.00007700
	N3	1.47137600	0.52258100	0.00055500
	C4	0.26720600	−0.13807500	−0.00127600
	N5	0.55138700	−1.45154400	−0.00282800
	N6	−0.84142100	0.64269300	−0.00277100
	C7	1.72226000	1.94519700	0.00298900
	N8	−2.05277700	0.05897300	0.00028300
	O9	−3.02371300	0.84619000	−0.00418400

	O10	−2.20279300	−1.17448400	0.00740700
	H11	0.75268400	2.44088200	0.00194300
	H12	2.28606900	2.23075300	0.89503200
	H13	2.28921300	2.23318000	−0.88626600

SCF Done: E(B3LYP, cation) = −314.0656767 a.u.

SCF Done: E(B3LYP, anion) = −557.0437665 a.u.

Table S87: Salt 87

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.67468300	0.00935200	−0.00001100
	N2	0.12778500	−1.06305900	0.00037200
	N3	1.46009600	−0.72163800	−0.00059300
	C4	1.46120000	0.56763800	0.00028800
	N5	0.16620400	1.07016600	−0.00002300
	N6	−2.00636100	0.03613400	−0.00011800
	H7	−0.13122800	−2.04067600	0.00063500
	H8	2.34086100	1.19145000	0.00034700
	H9	−0.09999700	2.04618100	0.00021400
	H10	−2.54623400	−0.81626400	0.00015500
	H11	−2.51656700	0.90615400	−0.00048200
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −298.0636709 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S88: Salt 88

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	1.13908000	1.02887800	0.00012700
	N2	1.84297800	−0.02428100	−0.00001800
	N3	0.98945400	−1.07733700	−0.00006300
	C4	−0.28251500	−0.66614700	0.00001400
	N5	−0.17767500	0.66418700	−0.00002000

	C6	−1.21991400	1.70107100	−0.00005700
	C7	−1.50611900	−1.50347000	0.00004900
	H8	1.35542800	−2.02391100	−0.00020800
	H9	−2.19481100	1.21927500	−0.00039900
	H10	−1.10178000	2.31242300	0.89333900
	H11	−1.10134100	2.31279800	−0.89313600
	H12	−1.24471600	−2.56122200	−0.00017600
	H13	−2.10903400	−1.29425900	0.88730100
	H14	−2.10930800	−1.29395100	−0.88694100
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −337.3360546 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S89: Salt 89

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.47534100	−0.62785300	0.00003000
	N2	−1.47587000	0.62752200	−0.00006500
	N3	−0.17047500	1.05257900	0.00004300
	C4	0.66687500	0.00044000	0.00000300
	N5	−0.17063300	−1.05243600	−0.00001100
	N6	1.99178000	−0.00011800	−0.00001900
	H7	0.03292400	2.04532000	0.00005500
	H8	0.03343500	−2.04505300	0.00011200
	H9	2.51851900	0.86180900	0.00006500
	H10	2.51764600	−0.86257100	−0.00009200
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −314.0552154 a.u.
SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S90: Salt 90

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.95084300	−1.17263000	−0.00095200
	N2	1.79153100	−0.22542300	0.00058800
	N3	1.10330500	0.94038700	0.00025100
	C4	−0.22970700	0.71021600	−0.00009100
	N5	−0.30366700	−0.62651500	−0.00007800
	N6	−1.38823800	−1.44672200	0.00003000
	N7	−1.22440700	1.60185200	−0.00028100
	H8	1.60344900	1.82132800	0.00070400
	H9	−1.18849000	−2.43403400	0.00065800
	H10	−2.31486600	−1.06327600	0.00306000
	H11	−2.19333300	1.32523000	−0.00046100
	H12	−1.03408900	2.59281600	−0.00032600
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −369.3807307 a.u.
SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S91: Salt 91

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800
	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200

	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S92: Salt 92

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.71309600	1.63579100	0.00000000
	C2	0.00000000	0.49075400	0.00000000
	N3	1.34087600	0.55400700	0.00000000
	N4	−0.63397000	−0.66964200	0.00000000
	N5	−0.05044100	−1.92877000	0.00000000
	H6	−1.72036800	1.63935700	0.00000000
	H7	−0.25478500	2.53240900	0.00000000
	H8	1.92947100	−0.26070500	0.00000000
	H9	1.81369600	1.44397200	0.00000000
	H10	−1.64306300	−0.68139000	0.00000000
	H11	−0.67178300	−2.71571000	0.00000000
	H12	0.94325200	−2.04216900	0.00000000
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000

	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S93: Salt 93

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.00000000	2.42944600	−0.09893800
	N2	0.00000000	1.14998700	−0.65450900
	C3	0.00000000	0.00000000	0.02528500
	N4	0.00000000	−1.14998700	−0.65450900
	N5	0.00000000	−2.42944600	−0.09893800
	N6	0.00000000	0.00000000	1.37233500
	H7	0.00000000	3.19851000	−0.74127800
	H8	0.00000000	2.56996300	0.89042200
	H9	0.00000000	1.13876300	−1.66204000
	H10	0.00000000	−1.13876300	−1.66204000
	H11	0.00000000	−3.19851000	−0.74127800
	H12	0.00000000	−2.56996300	0.89042200
	H13	0.00000000	−0.84963300	1.90800300
	H14	0.00000000	0.84963300	1.90800300
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000

	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −316.4385003 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S94: Salt 94

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.26743958	−0.76210486	−0.11251109
	C2	−0.27680858	0.11490214	0.09680091
	N3	−2.62460158	−0.63154486	0.22361791
	N4	0.99154442	−0.35337886	0.08387891
	N5	2.06350642	0.54806814	0.11087491
	N6	−0.45997458	1.42000114	0.32222491
	N7	−1.63937558	2.07287214	−0.08446609
	H8	−1.02863758	−1.65502386	−0.52334309
	H9	−2.73284058	−0.61934086	1.23390591
	H10	−2.99096558	0.22618414	−0.17552609
	H11	1.15006942	−1.34982986	0.17710691
	H12	1.29594258	1.19219586	0.27820109
	H13	2.62334342	0.40968814	0.94722791
	H14	2.64196342	0.43870114	−0.71719109
	H15	−1.96709158	2.66545914	0.67256191
	H16	−1.44770758	2.64882414	−0.90086409
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −371.8407102 a.u.
SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S95: Salt 95

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	2.31218400	0.76862300	0.00000000
	C2	1.20229600	0.02255600	0.00000000
	N3	0.00000000	0.66359500	0.00000000
	N4	1.26145600	−1.29536300	0.00000000
	C5	−1.27820400	0.00713000	0.00000000
	N6	−2.32216300	0.85491600	0.00000000
	O7	−1.35801900	−1.20338400	0.00000000
	H8	3.22630700	0.34135400	0.00000000
	H9	2.28234200	1.77628500	0.00000000
	H10	0.02372300	1.67372500	0.00000000
	H11	0.37690600	−1.80805400	0.00000000
	H12	2.14512200	−1.78250700	0.00000000
	H13	−3.24569300	0.44611200	0.00000000
	H14	−2.24945800	1.85963800	0.00000000
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −374.5987024 a.u.
SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S96: Salt 96

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.23126100	−0.61392200	−0.00005700
	C2	−0.06944600	0.01029100	−0.00002200
	N3	−2.41564800	0.10939600	−0.00009600
	N4	1.12200500	−0.76734500	0.00008400
	N5	2.24162600	0.08278500	0.00006100
	O6	0.09192400	1.23885400	0.00003400
	H7	−1.31636200	−1.61920200	−0.00004200
	H8	−3.27674900	−0.40124900	−0.00008900
	H9	−2.33833700	1.11046000	−0.00012000
	H10	1.25457300	−1.76698500	0.00002500
	H11	1.70267300	1.03124200	0.00000300
	H12	2.81920300	−0.00159200	0.84339400
	H13	2.81922300	−0.00165200	−0.84325300
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −336.3373235 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S97: Salt 97

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.39033800	1.87880800	−0.00009500
	C2	−0.65775000	0.58470300	−0.00009100
	N3	−1.99058900	0.17360200	0.00015500
	N4	−2.14178400	−1.22860500	0.00000100
	N5	0.13883600	−0.46530000	−0.00009200

	N6	1.54801100	−0.32932400	0.00002000
	O7	2.14711400	−1.37170000	−0.00003100
	O8	2.02664500	0.80094200	0.00014300
	H9	0.58973600	2.14741300	−0.00025000
	H10	−1.11132200	2.58517400	0.00002500
	H11	−2.80652400	0.76708000	0.00022100
	H12	−1.05236600	−1.48783800	−0.00041100
	H13	−2.60580500	−1.57923800	0.84408800
	H14	−2.60623400	−1.57900700	−0.84394600
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −465.6555662 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S98: Salt 98

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.63151800	−1.53175700	0.00017900
	N2	−0.63750600	−1.53002600	−0.00069800
	N3	−1.05571500	−0.23777700	0.00005900
	C4	0.00062000	0.58293300	−0.00017600
	N5	1.05612100	−0.24001700	0.00002300
	C6	2.49454500	0.06414800	0.00026300
	C7	0.00297500	2.06623300	−0.00026200
	C8	−2.49346800	0.06453600	0.00041600
	H9	3.01255800	−0.89198200	0.00052200
	H10	2.75264700	0.62484100	−0.89737600
	H11	2.75226100	0.62510600	0.89784600

	H12	1.02206200	2.44947700	−0.00006000
	H13	−0.50977200	2.44820700	−0.88677800
	H14	−0.51016600	2.44831600	0.88597600
	H15	−2.62545000	1.14379800	0.00106400
	H16	−2.94165000	−0.36839200	−0.89268300
	H17	−2.94145100	−0.36943600	0.89310700
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −376.6673328 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S99: Salt 99

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.60584700	−1.52255200	0.00008900
	N2	−0.65427800	−1.50393700	−0.00028300
	N3	−1.07049400	−0.19824200	0.00003200
	C4	0.00675400	0.60547600	−0.00006000
	N5	1.06035500	−0.23187400	−0.00001500
	C6	2.49252300	0.07273700	0.00010900
	N7	0.04688700	1.93796900	−0.00011200
	C8	−2.50303000	0.11401600	0.00015500
	H9	3.01461000	−0.88165800	0.00024300
	H10	2.75697800	0.63012500	−0.89975200
	H11	2.75677200	0.63026100	0.89994600
	H12	−0.79576700	2.49123100	−0.00002800
	H13	0.92630800	2.43182100	−0.00019300
	H14	−2.63741500	1.19426500	0.00067300

	H15	−2.95858400	−0.30906800	−0.89398900
	H16	−2.95859700	−0.30990500	0.89389500
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −392.7171077 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S100: Salt 100

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.93563500	−0.44076800	1.10484500
	C2	−1.23017700	1.06824900	0.78225000
	N3	−0.03668700	1.49735700	0.11426700
	C4	0.93779000	0.51701700	0.10567000
	N5	0.39582300	−0.63018600	0.61295000
	N6	−1.98026300	−1.13838600	0.32629600
	C7	−2.74428200	−0.29187600	−0.36956600
	N8	−2.41956500	0.97595600	−0.09283900
	N9	−3.71245800	−0.65796400	−1.20204100
	N10	2.11750100	0.81141500	−0.34160500
	N11	3.09401000	−0.20931600	−0.31432000
	O12	4.12378300	0.06300600	−0.87523900
	O13	2.86243900	−1.27923500	0.27060200
	H14	−1.03465800	−0.70595400	2.15770800
	H15	−1.47438000	1.67616500	1.65352200
	H16	0.25814600	2.46303400	0.08001700
	H17	1.03230300	−1.38354100	0.85526100
	H18	−2.05280800	−2.14382800	0.27536900

	H19	−2.79488200	1.77163400	−0.58804200
	H20	−4.27963800	0.02517500	−1.68129500
	H21	−3.91855700	−1.63071700	−1.37358600
Anion	N1	−2.61644400	−2.70900200	0.00000000
	N2	−1.36097900	−3.10512500	0.00000000
	N3	−0.53208100	−2.03354200	0.00000000
	C4	−1.37410600	−1.01060100	0.00000000
	N5	−2.66455800	−1.36581900	0.00000000
	N6	−1.11669900	0.37771600	0.00000000
	C7	0.00000000	1.13043900	0.00000000
	N8	−0.20677100	2.47584100	0.00000000
	N9	1.18230100	0.50638500	0.00000000
	N10	2.32550500	1.23860400	0.00000000
	O11	3.36905500	0.59625800	0.00000000
	O12	2.34069800	2.50334500	0.00000000
	H13	−1.99470100	0.87833500	0.00000000
	H14	0.62593000	3.05339800	0.00000000
	H15	−1.13653800	2.85700400	0.00000000

SCF Done: E(B3LYP, cation) = −690.819319 a.u.

SCF Done: E(B3LYP, anion) = −666.5842593 a.u.

Table S101: Salt 101

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.00001200	0.00000000	0.00000000
	H2	0.09263200	0.83857300	−0.58434300
	H3	0.10779100	−0.83730900	−0.58355400
	H4	0.72571300	0.00690600	0.72562600
	H5	−0.92605200	−0.00816900	0.44227100
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000

	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −56.9203571 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S102: Salt 102

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.16030900	1.13421300	0.00001100
	N2	0.64022800	0.00541000	−0.00001400
	C3	−0.14235700	−1.07565000	0.00000300
	N4	−1.41450500	−0.66298500	0.00000500
	C5	−1.45516100	0.71501800	−0.00000800
	C6	2.11612700	−0.00840000	0.00000300
	H7	0.25356300	2.12801300	0.00001300
	H8	0.19084100	−2.10049900	−0.00000100
	H9	−2.21768000	−1.27914800	0.00000700
	H10	−2.37804200	1.26900300	−0.00001200
	H11	2.46634300	1.02069300	−0.00026000
	H12	2.47754500	−0.51284000	0.89485800
	H13	2.47756200	−0.51328600	−0.89459400
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −265.9810056 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S103: Salt 103

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.65541700	−0.00411800	0.00005100

	N2	−0.75045600	−0.00232700	−0.00003900
	H3	0.99718400	0.96411800	−0.00012100
	H4	1.05415400	−0.45557600	0.83700000
	H5	1.05425800	−0.45589200	−0.83667700
	H6	−1.21844400	−0.89213100	−0.00011000
	H7	−1.22187800	0.88459500	−0.00017400
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −112.2418137 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S104: Salt 104

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800
	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200
	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700

	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S105: Salt 105

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.71309600	1.63579100	0.00000000
	C2	0.00000000	0.49075400	0.00000000
	N3	1.34087600	0.55400700	0.00000000
	N4	−0.63397000	−0.66964200	0.00000000
	N5	−0.05044100	−1.92877000	0.00000000
	H6	−1.72036800	1.63935700	0.00000000
	H7	−0.25478500	2.53240900	0.00000000
	H8	1.92947100	−0.26070500	0.00000000
	H9	1.81369600	1.44397200	0.00000000
	H10	−1.64306300	−0.68139000	0.00000000
	H11	−0.67178300	−2.71571000	0.00000000
	H12	0.94325200	−2.04216900	0.00000000
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S106: Salt 106

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.00000000	2.42944600	−0.09893800
	N2	0.00000000	1.14998700	−0.65450900
	C3	0.00000000	0.00000000	0.02528500
	N4	0.00000000	−1.14998700	−0.65450900
	N5	0.00000000	−2.42944600	−0.09893800
	N6	0.00000000	0.00000000	1.37233500
	H7	0.00000000	3.19851000	−0.74127800
	H8	0.00000000	2.56996300	0.89042200
	H9	0.00000000	1.13876300	−1.66204000
	H10	0.00000000	−1.13876300	−1.66204000
	H11	0.00000000	−3.19851000	−0.74127800
	H12	0.00000000	−2.56996300	0.89042200
	H13	0.00000000	−0.84963300	1.90800300
	H14	0.00000000	0.84963300	1.90800300
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −316.4385003 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S107: Salt 107

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.73090600	1.42465800	0.00000000
	C2	0.00000000	0.28737400	0.00000000
	N3	1.33364100	0.45849100	0.00000000

	N4	−0.65902100	−0.87579600	0.00000000
	N5	2.38734200	−0.46354400	0.00000000
	N6	−0.19531500	−2.19352200	0.00000000
	N7	−2.12655000	1.51794100	0.00000000
	H8	−0.26473700	2.31587700	0.00000000
	H9	1.66735400	1.40846300	0.00000000
	H10	−1.66209300	−0.83875500	0.00000000
	H11	3.30922600	−0.07173500	0.00000000
	H12	2.24095500	−1.44742300	0.00000000
	H13	−0.89921200	−2.90635300	0.00000000
	H14	0.77363900	−2.41899000	0.00000000
	H15	−2.51076700	2.44330700	0.00000000
	H16	−2.71870400	0.71376600	0.00000000
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −371.7391764 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S108: Salt 108

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	2.31218400	0.76862300	0.00000000
	C2	1.20229600	0.02255600	0.00000000
	N3	0.00000000	0.66359500	0.00000000
	N4	1.26145600	−1.29536300	0.00000000
	C5	−1.27820400	0.00713000	0.00000000
	N6	−2.32216300	0.85491600	0.00000000
	O7	−1.35801900	−1.20338400	0.00000000
	H8	3.22630700	0.34135400	0.00000000
	H9	2.28234200	1.77628500	0.00000000

	H10	0.02372300	1.67372500	0.00000000
	H11	0.37690600	−1.80805400	0.00000000
	H12	2.14512200	−1.78250700	0.00000000
	H13	−3.24569300	0.44611200	0.00000000
	H14	−2.24945800	1.85963800	0.00000000
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −374.5987024 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S109: Salt 109

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−2.30865200	0.81588100	0.00000000
	C2	−1.21694900	0.03718400	0.00000000
	N3	0.00000000	0.64962600	0.00000000
	N4	−1.29726400	−1.27578000	0.00000000
	C5	1.27171000	0.00451000	0.00000000
	N6	2.30605800	0.88525700	0.00000000
	N7	1.30701300	−1.27093700	0.00000000
	H8	−3.23217400	0.41098700	0.00000000
	H9	−2.25308100	1.82198600	0.00000000
	H10	−0.00498400	1.65842700	0.00000000
	H11	−0.38525300	−1.77463900	0.00000000
	H12	−2.18726700	−1.75083000	0.00000000
	H13	3.25154100	0.53751900	0.00000000
	H14	2.19157500	1.88552200	0.00000000
	H15	2.24099900	−1.66747000	0.00000000
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600

	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −354.7051979 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S110: Salt 110

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.23126100	−0.61392200	−0.00005700
	C2	−0.06944600	0.01029100	−0.00002200
	N3	−2.41564800	0.10939600	−0.00009600
	N4	1.12200500	−0.76734500	0.00008400
	N5	2.24162600	0.08278500	0.00006100
	O6	0.09192400	1.23885400	0.00003400
	H7	−1.31636200	−1.61920200	−0.00004200
	H8	−3.27674900	−0.40124900	−0.00008900
	H9	−2.33833700	1.11046000	−0.00012000
	H10	1.25457300	−1.76698500	0.00002500
	H11	1.70267300	1.03124200	0.00000300
	H12	2.81920300	−0.00159200	0.84339400
	H13	2.81922300	−0.00165200	−0.84325300
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000

	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −336.3373235 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S111: Salt 111

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.59451600	1.20187700	−0.00003200
	N2	0.70987100	1.21521700	−0.00001400
	N3	1.06725400	−0.09451300	0.00000000
	C4	0.00077400	−0.88021700	−0.00013000
	N5	−1.08025000	−0.08242400	−0.00002500
	C6	−2.49413600	−0.50489600	0.00008000
	C7	2.48650600	−0.47089700	0.00007100
	H8	−1.22032700	2.08055400	−0.00001100
	H9	−0.00234600	−1.95863900	−0.00020400
	H10	−3.11391800	0.38900000	0.00000800
	H11	−2.70184400	−1.08933900	−0.89524100
	H12	−2.70178700	−1.08916200	0.89553200
	H13	2.55902600	−1.55669300	0.00020400
	H14	2.95566400	−0.05954800	−0.89231300
	H15	2.95564100	−0.05933200	0.89236600
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −321.329351 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S112: Salt 112

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.63151800	−1.53175700	0.00017900
	N2	−0.63750600	−1.53002600	−0.00069800
	N3	−1.05571500	−0.23777700	0.00005900
	C4	0.00062000	0.58293300	−0.00017600
	N5	1.05612100	−0.24001700	0.00002300
	C6	2.49454500	0.06414800	0.00026300
	C7	0.00297500	2.06623300	−0.00026200
	C8	−2.49346800	0.06453600	0.00041600
	H9	3.01255800	−0.89198200	0.00052200
	H10	2.75264700	0.62484100	−0.89737600
	H11	2.75226100	0.62510600	0.89784600
	H12	1.02206200	2.44947700	−0.00006000
	H13	−0.50977200	2.44820700	−0.88677800
	H14	−0.51016600	2.44831600	0.88597600
	H15	−2.62545000	1.14379800	0.00106400
	H16	−2.94165000	−0.36839200	−0.89268300
	H17	−2.94145100	−0.36943600	0.89310700
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −376.6673328 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 A.U

Table S113: Salt 113

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.60584700	−1.52255200	0.00008900
	N2	−0.65427800	−1.50393700	−0.00028300

	N3	−1.07049400	−0.19824200	0.00003200
	C4	0.00675400	0.60547600	−0.00006000
	N5	1.06035500	−0.23187400	−0.00001500
	C6	2.49252300	0.07273700	0.00010900
	N7	0.04688700	1.93796900	−0.00011200
	C8	−2.50303000	0.11401600	0.00015500
	H9	3.01461000	−0.88165800	0.00024300
	H10	2.75697800	0.63012500	−0.89975200
	H11	2.75677200	0.63026100	0.89994600
	H12	−0.79576700	2.49123100	−0.00002800
	H13	0.92630800	2.43182100	−0.00019300
	H14	−2.63741500	1.19426500	0.00067300
	H15	−2.95858400	−0.30906800	−0.89398900
	H16	−2.95859700	−0.30990500	0.89389500
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −392.7171077 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S114: Salt 114

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−0.67569800	0.42810400	−1.21284500
	C2	0.69084800	0.98423600	−0.83358600
	N3	1.50822200	0.00317200	0.00559000
	C4	0.67576900	−0.42786800	1.21290300
	C5	−0.69082100	−0.98410200	0.83384700
	N6	−1.50835400	−0.00320300	−0.00556300
	N7	−2.73768500	−0.67633900	−0.35499600
	N8	−1.97373700	1.18092400	0.68413700

	N9	2.73807600	0.67601800	0.35473700
	N10	1.97338600	−1.18101900	−0.68427700
	H11	−0.60085700	−0.44934200	−1.85746400
	H12	−1.24740700	1.19668900	−1.73392700
	H13	1.27182300	1.19844600	−1.73153400
	H14	0.61444600	1.90982700	−0.25969200
	H15	0.60090000	0.44967900	1.85739000
	H16	1.24743700	−1.19638200	1.73413900
	H17	−1.27179300	−1.19813300	1.73183000
	H18	−0.61444900	−1.90981200	0.26015200
	H19	−2.53680000	−1.49154200	−0.93190700
	H20	−3.31871800	−0.01503500	−0.87267700
	H21	−1.20653000	1.65625400	1.15106500
	H22	−2.66217800	0.87606400	1.37422200
	H23	2.53725300	1.49157500	0.93123700
	H24	3.31831300	0.01469300	0.87334700
	H25	1.20624700	−1.65593100	−1.15168700
	H26	2.66237800	−0.87613200	−1.37379700
Anion	N1	−0.36965900	2.81889800	0.00000000
	N2	0.94888300	2.68000500	0.00000000
	N3	1.26302000	1.37463600	0.00000000
	C4	0.07711200	0.73207500	0.00000000
	N5	−0.94888300	1.60762500	0.00000000
	C6	−0.07711200	−0.73207500	0.00000000
	N7	−1.26302000	−1.37463600	0.00000000
	N8	−0.94888300	−2.68000500	0.00000000
	N9	0.36965900	−2.81889800	0.00000000
	N10	0.94888300	−1.60762500	0.00000000

SCF Done: E(B3LYP, cation) = −489.9479396 a.u.

SCF Done: E(B3LYP, anion) = −514.2825578 a.u.

Table S115: Salt 115

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.65541700	−0.00411800	0.00005100
	N2	−0.75045600	−0.00232700	−0.00003900
	H3	0.99718400	0.96411800	−0.00012100
	H4	1.05415400	−0.45557600	0.83700000
	H5	1.05425800	−0.45589200	−0.83667700
	H6	−1.21844400	−0.89213100	−0.00011000
	H7	−1.22187800	0.88459500	−0.00017400

Anion	C1	0.00000000	0.37938600	0.00000000
	N2	−0.42855600	1.63963700	0.00000000
	N3	−1.77005300	1.50771800	0.00000000
	N4	−2.09637900	0.22834300	0.00000000
	N5	−0.97985900	−0.52614600	0.00000000
	N6	1.38152500	0.07435500	0.00000000
	N7	1.71473300	−1.10429000	0.00000000
	N8	2.17859000	−2.14480400	0.00000000

SCF Done: E(B3LYP, cation) = −112.2418137 a.u.

SCF Done: E(B3LYP, anion) = −421.4323883 a.u.

Table S116: Salt 116

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.00001200	0.00000000	0.00000000
	H2	0.09263200	0.83857300	−0.58434300
	H3	0.10779100	−0.83730900	−0.58355400
	H4	0.72571300	0.00690600	0.72562600
	H5	−0.92605200	−0.00816900	0.44227100
Anion	C1	0.00000000	0.37938600	0.00000000
	N2	−0.42855600	1.63963700	0.00000000
	N3	−1.77005300	1.50771800	0.00000000
	N4	−2.09637900	0.22834300	0.00000000
	N5	−0.97985900	−0.52614600	0.00000000
	N6	1.38152500	0.07435500	0.00000000
	N7	1.71473300	−1.10429000	0.00000000
	N8	2.17859000	−2.14480400	0.00000000

SCF Done: E(B3LYP, cation) = −56.9203571 a.u.

SCF Done: E(B3LYP, anion) = −421.4323883 a.u.

Table S117: Salt 117

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800

	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200
	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	C1	0.00000000	0.37938600	0.00000000
	N2	−0.42855600	1.63963700	0.00000000
	N3	−1.77005300	1.50771800	0.00000000
	N4	−2.09637900	0.22834300	0.00000000
	N5	−0.97985900	−0.52614600	0.00000000
	N6	1.38152500	0.07435500	0.00000000
	N7	1.71473300	−1.10429000	0.00000000
	N8	2.17859000	−2.14480400	0.00000000

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −421.4323883 a.u.

Table S118: Salt 118

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.71309600	1.63579100	0.00000000
	C2	0.00000000	0.49075400	0.00000000
	N3	1.34087600	0.55400700	0.00000000
	N4	−0.63397000	−0.66964200	0.00000000
	N5	−0.05044100	−1.92877000	0.00000000
	H6	−1.72036800	1.63935700	0.00000000
	H7	−0.25478500	2.53240900	0.00000000
	H8	1.92947100	−0.26070500	0.00000000
	H9	1.81369600	1.44397200	0.00000000
	H10	−1.64306300	−0.68139000	0.00000000
	H11	−0.67178300	−2.71571000	0.00000000
	H12	0.94325200	−2.04216900	0.00000000
Anion	C1	0.00000000	0.37938600	0.00000000
	N2	−0.42855600	1.63963700	0.00000000
	N3	−1.77005300	1.50771800	0.00000000
	N4	−2.09637900	0.22834300	0.00000000
	N5	−0.97985900	−0.52614600	0.00000000
	N6	1.38152500	0.07435500	0.00000000
	N7	1.71473300	−1.10429000	0.00000000

	N8	2.17859000	−2.14480400	0.00000000

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −421.4323883 a.u.

Table S119: Salt 119

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.73873200	−1.43272900	0.06523700
	C2	2.78115000	−0.53199600	−0.09618600
	C3	2.58272300	0.83836400	−0.08296900
	C4	1.28876100	1.30925800	0.08646600
	C5	0.18564400	0.45946600	0.27650200
	C6	0.47216300	−0.91411900	0.27061800
	C7	−1.19631900	0.94965900	0.46912400
	N8	−2.13865200	0.28782100	−0.07950600
	N9	−3.42660700	0.69305100	0.12274000
	C10	−4.41899100	−0.09219600	−0.35406800
	N11	−5.68230800	0.33106500	−0.24703800
	N12	−4.11616000	−1.25828800	−0.90322900
	N13	−0.62189000	−1.88684500	0.53065600
	O14	−1.07337100	−1.92087600	1.65905600
	O15	−0.98524100	−2.57172500	−0.41467900
	N16	1.09775600	2.78355000	0.00382200
	O17	−0.03649000	3.18356500	−0.24463100
	O18	2.07313700	3.48293000	0.17674500
	N19	4.16165300	−1.06148900	−0.30003200
	O20	5.04731300	−0.23940300	−0.44505100
	O21	4.28523500	−2.27384100	−0.30307900
	H22	1.92627500	−2.49880100	0.04810600
	H23	3.40941000	1.52275400	−0.21875300
	H24	−1.36434000	1.83442100	1.07924800
	H25	−3.64335000	1.52660700	0.66309300
	H26	−6.45564100	−0.26488200	−0.50002900
	H27	−5.90473400	1.26755400	0.05394700
	H28	−4.81945600	−1.83307300	−1.34151400
	H29	−3.15254800	−1.57608700	−0.91123000
Anion	C1	1.18847300	1.30965400	0.00000000
	N2	2.44302700	0.81478800	0.00000000
	N3	3.22740900	1.89149100	0.00000000
	N4	2.47494200	2.99969600	0.00000000
	N5	1.18847300	2.65915100	0.00000000

	N6	−0.03688000	0.62878200	0.00000000
	N7	0.03688000	−0.62878200	0.00000000
	C8	−1.18847300	−1.30965400	0.00000000
	N9	−2.44302700	−0.81478800	0.00000000
	N10	−3.22740900	−1.89149100	0.00000000
	N11	−2.47494200	−2.99969600	0.00000000
	N12	−1.18847300	−2.65915100	0.00000000

SCF Done: E(B3LYP, cation) = −1144.0380666 a.u.

SCF Done: E(B3LYP, anion) = −623.7876564 a.u.

Table S120: Salt 120

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.73873200	−1.43272900	0.06523700
	C2	2.78115000	−0.53199600	−0.09618600
	C3	2.58272300	0.83836400	−0.08296900
	C4	1.28876100	1.30925800	0.08646600
	C5	0.18564400	0.45946600	0.27650200
	C6	0.47216300	−0.91411900	0.27061800
	C7	−1.19631900	0.94965900	0.46912400
	N8	−2.13865200	0.28782100	−0.07950600
	N9	−3.42660700	0.69305100	0.12274000
	C10	−4.41899100	−0.09219600	−0.35406800
	N11	−5.68230800	0.33106500	−0.24703800
	N12	−4.11616000	−1.25828800	−0.90322900
	N13	−0.62189000	−1.88684500	0.53065600
	O14	−1.07337100	−1.92087600	1.65905600
	O15	−0.98524100	−2.57172500	−0.41467900
	N16	1.09775600	2.78355000	0.00382200
	O17	−0.03649000	3.18356500	−0.24463100
	O18	2.07313700	3.48293000	0.17674500
	N19	4.16165300	−1.06148900	−0.30003200
	O20	5.04731300	−0.23940300	−0.44505100
	O21	4.28523500	−2.27384100	−0.30307900
	H22	1.92627500	−2.49880100	0.04810600
	H23	3.40941000	1.52275400	−0.21875300
	H24	−1.36434000	1.83442100	1.07924800
	H25	−3.64335000	1.52660700	0.66309300
	H26	−6.45564100	−0.26488200	−0.50002900
	H27	−5.90473400	1.26755400	0.05394700
	H28	−4.81945600	−1.83307300	−1.34151400

	H29	−3.15254800	−1.57608700	−0.91123000
Anion	N1	−3.97109800	−1.75691000	1.87261300
	N2	−2.98430100	−1.03901700	1.33777000
	C3	−3.60589500	−0.19915300	0.49279600
	N4	−4.94010300	−0.37919200	0.48746600
	N5	−5.13769100	−1.36719600	1.35956200
	C6	−2.91663900	0.79966300	−0.30367000
	N7	−3.49857500	1.89095200	−0.74118100
	O8	−2.53466200	2.56555700	−1.48307000
	N9	−1.34649500	1.90459000	−1.48073500
	C10	−1.54382200	0.82814500	−0.76292100
	N11	−0.59307300	−0.20001700	−0.64757200
	N12	0.59309300	0.20049800	−0.64776100
	C13	1.54379900	−0.82777700	−0.76327000
	C14	2.91666100	−0.79952000	−0.30413200
	N15	3.49840900	−1.89089800	−0.74166000
	O16	2.53422700	−2.56539200	−1.48347400
	N17	1.34622000	−1.90424100	−1.48096800
	C18	3.60606800	0.19911300	0.49241600
	N19	4.94048900	0.37781200	0.48864000
	N20	5.13801500	1.36599300	1.36052800
	N21	3.97113100	1.75706800	1.87205000
	N22	2.98432700	1.03996500	1.33625200

SCF Done: E(B3LYP, cation) = −1144.0380666 a.u.

SCF Done: E(B3LYP, anion) = −1145.6620709 a.u.

Table S121: Salt 121

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.73873200	−1.43272900	0.06523700
	C2	2.78115000	−0.53199600	−0.09618600
	C3	2.58272300	0.83836400	−0.08296900
	C4	1.28876100	1.30925800	0.08646600
	C5	0.18564400	0.45946600	0.27650200
	C6	0.47216300	−0.91411900	0.27061800
	C7	−1.19631900	0.94965900	0.46912400
	N8	−2.13865200	0.28782100	−0.07950600
	N9	−3.42660700	0.69305100	0.12274000
	C10	−4.41899100	−0.09219600	−0.35406800
	N11	−5.68230800	0.33106500	−0.24703800
	N12	−4.11616000	−1.25828800	−0.90322900

	N13	−0.62189000	−1.88684500	0.53065600
	O14	−1.07337100	−1.92087600	1.65905600
	O15	−0.98524100	−2.57172500	−0.41467900
	N16	1.09775600	2.78355000	0.00382200
	O17	−0.03649000	3.18356500	−0.24463100
	O18	2.07313700	3.48293000	0.17674500
	N19	4.16165300	−1.06148900	−0.30003200
	O20	5.04731300	−0.23940300	−0.44505100
	O21	4.28523500	−2.27384100	−0.30307900
	H22	1.92627500	−2.49880100	0.04810600
	H23	3.40941000	1.52275400	−0.21875300
	H24	−1.36434000	1.83442100	1.07924800
	H25	−3.64335000	1.52660700	0.66309300
	H26	−6.45564100	−0.26488200	−0.50002900
	H27	−5.90473400	1.26755400	0.05394700
	H28	−4.81945600	−1.83307300	−1.34151400
	H29	−3.15254800	−1.57608700	−0.91123000
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −1144.0380666 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S122: Salt 122

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.73873200	−1.43272900	0.06523700
	C2	2.78115000	−0.53199600	−0.09618600
	C3	2.58272300	0.83836400	−0.08296900
	C4	1.28876100	1.30925800	0.08646600
	C5	0.18564400	0.45946600	0.27650200
	C6	0.47216300	−0.91411900	0.27061800
	C7	−1.19631900	0.94965900	0.46912400
	N8	−2.13865200	0.28782100	−0.07950600
	N9	−3.42660700	0.69305100	0.12274000
	C10	−4.41899100	−0.09219600	−0.35406800

	N11	−5.68230800	0.33106500	−0.24703800
	N12	−4.11616000	−1.25828800	−0.90322900
	N13	−0.62189000	−1.88684500	0.53065600
	O14	−1.07337100	−1.92087600	1.65905600
	O15	−0.98524100	−2.57172500	−0.41467900
	N16	1.09775600	2.78355000	0.00382200
	O17	−0.03649000	3.18356500	−0.24463100
	O18	2.07313700	3.48293000	0.17674500
	N19	4.16165300	−1.06148900	−0.30003200
	O20	5.04731300	−0.23940300	−0.44505100
	O21	4.28523500	−2.27384100	−0.30307900
	H22	1.92627500	−2.49880100	0.04810600
	H23	3.40941000	1.52275400	−0.21875300
	H24	−1.36434000	1.83442100	1.07924800
	H25	−3.64335000	1.52660700	0.66309300
	H26	−6.45564100	−0.26488200	−0.50002900
	H27	−5.90473400	1.26755400	0.05394700
	H28	−4.81945600	−1.83307300	−1.34151400
	H29	−3.15254800	−1.57608700	−0.91123000
Anion	C1	−0.32331000	0.09924700	0.00018400
	N2	0.18994600	1.32878300	0.00059600
	N3	1.49701900	1.17153100	−0.00033900
	N4	1.72208000	−0.18822300	−0.00011300
	N5	0.58879600	−0.88756000	0.00072200
	O6	2.87185800	−0.68467900	−0.00033400
	N7	−1.73407500	−0.14934000	−0.00034800
	O8	−2.11102300	−1.32486900	−0.00005500
	O9	−2.49914900	0.81932000	−0.00020200

SCF Done: E(B3LYP, cation) = −1144.0380666 a.u.

SCF Done: E(B3LYP, anion) = −537.5669456 a.u.

Table S123: Salt 123

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.73873200	−1.43272900	0.06523700
	C2	2.78115000	−0.53199600	−0.09618600
	C3	2.58272300	0.83836400	−0.08296900
	C4	1.28876100	1.30925800	0.08646600
	C5	0.18564400	0.45946600	0.27650200
	C6	0.47216300	−0.91411900	0.27061800
	C7	−1.19631900	0.94965900	0.46912400

	N8	−2.13865200	0.28782100	−0.07950600
	N9	−3.42660700	0.69305100	0.12274000
	C10	−4.41899100	−0.09219600	−0.35406800
	N11	−5.68230800	0.33106500	−0.24703800
	N12	−4.11616000	−1.25828800	−0.90322900
	N13	−0.62189000	−1.88684500	0.53065600
	O14	−1.07337100	−1.92087600	1.65905600
	O15	−0.98524100	−2.57172500	−0.41467900
	N16	1.09775600	2.78355000	0.00382200
	O17	−0.03649000	3.18356500	−0.24463100
	O18	2.07313700	3.48293000	0.17674500
	N19	4.16165300	−1.06148900	−0.30003200
	O20	5.04731300	−0.23940300	−0.44505100
	O21	4.28523500	−2.27384100	−0.30307900
	H22	1.92627500	−2.49880100	0.04810600
	H23	3.40941000	1.52275400	−0.21875300
	H24	−1.36434000	1.83442100	1.07924800
	H25	−3.64335000	1.52660700	0.66309300
	H26	−6.45564100	−0.26488200	−0.50002900
	H27	−5.90473400	1.26755400	0.05394700
	H28	−4.81945600	−1.83307300	−1.34151400
	H29	−3.15254800	−1.57608700	−0.91123000
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −1144.0380666 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S124: Salt 124

Cartesian coordinates

Atom	X	Y	Z

Cation	C1	1.73873200	−1.43272900	0.06523700
	C2	2.78115000	−0.53199600	−0.09618600
	C3	2.58272300	0.83836400	−0.08296900
	C4	1.28876100	1.30925800	0.08646600
	C5	0.18564400	0.45946600	0.27650200
	C6	0.47216300	−0.91411900	0.27061800
	C7	−1.19631900	0.94965900	0.46912400
	N8	−2.13865200	0.28782100	−0.07950600
	N9	−3.42660700	0.69305100	0.12274000
	C10	−4.41899100	−0.09219600	−0.35406800
	N11	−5.68230800	0.33106500	−0.24703800
	N12	−4.11616000	−1.25828800	−0.90322900
	N13	−0.62189000	−1.88684500	0.53065600
	O14	−1.07337100	−1.92087600	1.65905600
	O15	−0.98524100	−2.57172500	−0.41467900
	N16	1.09775600	2.78355000	0.00382200
	O17	−0.03649000	3.18356500	−0.24463100
	O18	2.07313700	3.48293000	0.17674500
	N19	4.16165300	−1.06148900	−0.30003200
	O20	5.04731300	−0.23940300	−0.44505100
	O21	4.28523500	−2.27384100	−0.30307900
	H22	1.92627500	−2.49880100	0.04810600
	H23	3.40941000	1.52275400	−0.21875300
	H24	−1.36434000	1.83442100	1.07924800
	H25	−3.64335000	1.52660700	0.66309300
	H26	−6.45564100	−0.26488200	−0.50002900
	H27	−5.90473400	1.26755400	0.05394700
	H28	−4.81945600	−1.83307300	−1.34151400
	H29	−3.15254800	−1.57608700	−0.91123000
Anion	N1	0.00875500	−0.68767200	−0.00008400
	C2	−1.04271900	0.15278000	0.00006800
	C3	−0.60820500	1.49561500	−0.00001000
	N4	0.72848700	1.49980500	−0.00013900
	C5	1.02289200	0.17449800	0.00021400
	N6	2.39809700	−0.28461200	0.00067900
	O7	3.29154400	0.56477300	−0.00031100
	O8	2.60950000	−1.49786000	−0.00025100
	N9	−2.39909000	−0.30038300	0.00022400
	O10	−3.28335800	0.57377800	−0.00011300
	O11	−2.64065600	−1.50622800	−0.00012600
	H12	−1.20179300	2.39696700	0.00003300

SCF Done: E(B3LYP, cation) = −1144.0380666 a.u.

SCF Done: E(B3LYP, anion) = −634.8962734 a.u.

Table S125: Salt 125

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.73873200	−1.43272900	0.06523700
	C2	2.78115000	−0.53199600	−0.09618600
	C3	2.58272300	0.83836400	−0.08296900
	C4	1.28876100	1.30925800	0.08646600
	C5	0.18564400	0.45946600	0.27650200
	C6	0.47216300	−0.91411900	0.27061800
	C7	−1.19631900	0.94965900	0.46912400
	N8	−2.13865200	0.28782100	−0.07950600
	N9	−3.42660700	0.69305100	0.12274000
	C10	−4.41899100	−0.09219600	−0.35406800
	N11	−5.68230800	0.33106500	−0.24703800
	N12	−4.11616000	−1.25828800	−0.90322900
	N13	−0.62189000	−1.88684500	0.53065600
	O14	−1.07337100	−1.92087600	1.65905600
	O15	−0.98524100	−2.57172500	−0.41467900
	N16	1.09775600	2.78355000	0.00382200
	O17	−0.03649000	3.18356500	−0.24463100
	O18	2.07313700	3.48293000	0.17674500
	N19	4.16165300	−1.06148900	−0.30003200
	O20	5.04731300	−0.23940300	−0.44505100
	O21	4.28523500	−2.27384100	−0.30307900
	H22	1.92627500	−2.49880100	0.04810600
	H23	3.40941000	1.52275400	−0.21875300
	H24	−1.36434000	1.83442100	1.07924800
	H25	−3.64335000	1.52660700	0.66309300
	H26	−6.45564100	−0.26488200	−0.50002900
	H27	−5.90473400	1.26755400	0.05394700
	H28	−4.81945600	−1.83307300	−1.34151400
	H29	−3.15254800	−1.57608700	−0.91123000
Anion	N1	−1.81120700	1.72418200	0.00000000
	N2	−0.79668000	2.57503900	0.00000000
	N3	0.35873200	1.89717100	0.00000000
	C4	0.00000000	0.58544800	0.00000000
	N5	−1.34623900	0.45662100	0.00000000
	N6	1.04723100	−0.34007800	0.00000000
	N7	0.81628700	−1.62454700	0.00000000
	O8	1.85074100	−2.38952400	0.00000000

	O9	−0.33534800	−2.15190100	0.00000000

SCF Done: E(B3LYP, cation) = −1144.0380666 a.u.

SCF Done: E(B3LYP, anion) = −517.0427728 a.u.

Table S126: Salt 126

Cartesian coordinates

	Atom	X	Y	Z
Cation	O1	−2.41721000	−1.63070300	0.00001300
	N2	−3.21717600	−0.34953200	0.00001200
	C3	−2.31548800	0.62805900	−0.00001500
	C4	−1.03473300	0.00120200	−0.00000200
	N5	−1.12730300	−1.31188400	−0.00003000
	O6	−4.41855900	−0.42314100	0.00002200
	C7	−2.72749400	2.06173600	−0.00003100
	C8	0.25640000	0.67453000	0.00002500
	N9	1.34268400	−0.00020500	0.00000800
	N10	2.52825500	0.68461500	0.00001700
	C11	3.66751000	−0.03976900	−0.00000100
	N12	4.84602300	0.59214800	0.00000500
	N13	3.57842000	−1.36176800	−0.00002100
	H14	−3.81569700	2.12749100	−0.00041800
	H15	−2.35725500	2.58076800	0.88829000
	H16	−2.35660700	2.58092500	−0.88798800
	H17	0.24820400	1.76774100	0.00004600
	H18	2.56191000	1.70080000	0.00003800
	H19	5.71362000	0.07824100	−0.00000200
	H20	4.91099100	1.59823400	0.00001800
	H21	4.39380900	−1.95431400	−0.00003700
	H22	2.65367600	−1.77728600	−0.00002200
Anion	N1	0.67195600	2.05851800	0.00000000
	N2	−0.67221000	2.05845700	0.00000000
	N3	−1.11928500	0.81026500	0.00000000
	C4	0.00000000	0.07854900	0.00000000
	N5	1.11920100	0.81038500	0.00000000
	N6	0.00008100	−1.36159900	0.00000000
	O7	1.08603400	−1.94390800	0.00000000
	O8	−1.08580900	−1.94402600	0.00000000

SCF Done: E(B3LYP, cation) = −674.7075741 a.u.

SCF Done: E(B3LYP, anion) = −462.3675711 a.u.

Table S127: Salt 127

Cartesian coordinates

	Atom	X	Y	Z
Cation	O1	−2.41721000	−1.63070300	0.00001300
	N2	−3.21717600	−0.34953200	0.00001200
	C3	−2.31548800	0.62805900	−0.00001500
	C4	−1.03473300	0.00120200	−0.00000200
	N5	−1.12730300	−1.31188400	−0.00003000
	O6	−4.41855900	−0.42314100	0.00002200
	C7	−2.72749400	2.06173600	−0.00003100
	C8	0.25640000	0.67453000	0.00002500
	N9	1.34268400	−0.00020500	0.00000800
	N10	2.52825500	0.68461500	0.00001700
	C11	3.66751000	−0.03976900	−0.00000100
	N12	4.84602300	0.59214800	0.00000500
	N13	3.57842000	−1.36176800	−0.00002100
	H14	−3.81569700	2.12749100	−0.00041800
	H15	−2.35725500	2.58076800	0.88829000
	H16	−2.35660700	2.58092500	−0.88798800
	H17	0.24820400	1.76774100	0.00004600
	H18	2.56191000	1.70080000	0.00003800
	H19	5.71362000	0.07824100	−0.00000200
	H20	4.91099100	1.59823400	0.00001800
	H21	4.39380900	−1.95431400	−0.00003700
	H22	2.65367600	−1.77728600	−0.00002200
Anion	C1	−0.32331000	0.09924700	0.00018400
	N2	0.18994600	1.32878300	0.00059600
	N3	1.49701900	1.17153100	−0.00033900
	N4	1.72208000	−0.18822300	−0.00011300
	N5	0.58879600	−0.88756000	0.00072200
	O6	2.87185800	−0.68467900	−0.00033400
	N7	−1.73407500	−0.14934000	−0.00034800
	O8	−2.11102300	−1.32486900	−0.00005500
	O9	−2.49914900	0.81932000	−0.00020200

SCF Done: E(B3LYP, cation) = −674.7075741 a.u.

SCF Done: E(B3LYP, anion) = −537.5669456 a.u.

Table S128: Salt 128

Cartesian coordinates

	Atom	X	Y	Z

Cation	O1	−2.41721000	−1.63070300	0.00001300
	N2	−3.21717600	−0.34953200	0.00001200
	C3	−2.31548800	0.62805900	−0.00001500
	C4	−1.03473300	0.00120200	−0.00000200
	N5	−1.12730300	−1.31188400	−0.00003000
	O6	−4.41855900	−0.42314100	0.00002200
	C7	−2.72749400	2.06173600	−0.00003100
	C8	0.25640000	0.67453000	0.00002500
	N9	1.34268400	−0.00020500	0.00000800
	N10	2.52825500	0.68461500	0.00001700
	C11	3.66751000	−0.03976900	−0.00000100
	N12	4.84602300	0.59214800	0.00000500
	N13	3.57842000	−1.36176800	−0.00002100
	H14	−3.81569700	2.12749100	−0.00041800
	H15	−2.35725500	2.58076800	0.88829000
	H16	−2.35660700	2.58092500	−0.88798800
	H17	0.24820400	1.76774100	0.00004600
	H18	2.56191000	1.70080000	0.00003800
	H19	5.71362000	0.07824100	−0.00000200
	H20	4.91099100	1.59823400	0.00001800
	H21	4.39380900	−1.95431400	−0.00003700
	H22	2.65367600	−1.77728600	−0.00002200
Anion	N1	2.80157900	0.71401300	−0.00000900
	N2	3.00370900	−0.59546200	0.00005600
	N3	1.83247700	−1.24297800	−0.00000500
	C4	0.91587000	−0.26585200	0.00000000
	N5	1.48783600	0.95606100	0.00002600
	C6	−0.52956300	−0.40499200	−0.00001700
	N7	−1.21858900	−1.51344400	−0.00004500
	O8	−2.54597900	−1.14967400	−0.00008600
	N9	−2.68894200	0.24496000	−0.00001000
	C10	−1.46557700	0.70561100	0.00001400
	N11	−1.10914400	2.01489800	0.00007000
	H12	−0.10936200	2.20889500	0.00007000
	H13	−1.80967200	2.73356000	0.00007100

SCF Done: E(B3LYP, cation) = −674.7075741 a.u.

SCF Done: E(B3LYP, anion) = −574.1182786 a.u.

Table S129: Salt 129

Cartesian coordinates

	Atom	X	Y	Z

Cation	O1	−2.41721000	−1.63070300	0.00001300
	N2	−3.21717600	−0.34953200	0.00001200
	C3	−2.31548800	0.62805900	−0.00001500
	C4	−1.03473300	0.00120200	−0.00000200
	N5	−1.12730300	−1.31188400	−0.00003000
	O6	−4.41855900	−0.42314100	0.00002200
	C7	−2.72749400	2.06173600	−0.00003100
	C8	0.25640000	0.67453000	0.00002500
	N9	1.34268400	−0.00020500	0.00000800
	N10	2.52825500	0.68461500	0.00001700
	C11	3.66751000	−0.03976900	−0.00000100
	N12	4.84602300	0.59214800	0.00000500
	N13	3.57842000	−1.36176800	−0.00002100
	H14	−3.81569700	2.12749100	−0.00041800
	H15	−2.35725500	2.58076800	0.88829000
	H16	−2.35660700	2.58092500	−0.88798800
	H17	0.24820400	1.76774100	0.00004600
	H18	2.56191000	1.70080000	0.00003800
	H19	5.71362000	0.07824100	−0.00000200
	H20	4.91099100	1.59823400	0.00001800
	H21	4.39380900	−1.95431400	−0.00003700
	H22	2.65367600	−1.77728600	−0.00002200
Anion	C1	0.00000000	0.37938600	0.00000000
	N2	−0.42855600	1.63963700	0.00000000
	N3	−1.77005300	1.50771800	0.00000000
	N4	−2.09637900	0.22834300	0.00000000
	N5	−0.97985900	−0.52614600	0.00000000
	N6	1.38152500	0.07435500	0.00000000
	N7	1.71473300	−1.10429000	0.00000000
	N8	2.17859000	−2.14480400	0.00000000

SCF Done: E(B3LYP, cation) = −674.7075741 a.u.

SCF Done: E(B3LYP, anion) = −421.4323883 a.u.

Table S130: Salt 130

Cartesian coordinates

	Atom	X	Y	Z
Cation	O1	−2.41721000	−1.63070300	0.00001300
	N2	−3.21717600	−0.34953200	0.00001200
	C3	−2.31548800	0.62805900	−0.00001500
	C4	−1.03473300	0.00120200	−0.00000200
	N5	−1.12730300	−1.31188400	−0.00003000

	O6	−4.41855900	−0.42314100	0.00002200
	C7	−2.72749400	2.06173600	−0.00003100
	C8	0.25640000	0.67453000	0.00002500
	N9	1.34268400	−0.00020500	0.00000800
	N10	2.52825500	0.68461500	0.00001700
	C11	3.66751000	−0.03976900	−0.00000100
	N12	4.84602300	0.59214800	0.00000500
	N13	3.57842000	−1.36176800	−0.00002100
	H14	−3.81569700	2.12749100	−0.00041800
	H15	−2.35725500	2.58076800	0.88829000
	H16	−2.35660700	2.58092500	−0.88798800
	H17	0.24820400	1.76774100	0.00004600
	H18	2.56191000	1.70080000	0.00003800
	H19	5.71362000	0.07824100	−0.00000200
	H20	4.91099100	1.59823400	0.00001800
	H21	4.39380900	−1.95431400	−0.00003700
	H22	2.65367600	−1.77728600	−0.00002200
Anion	N1	0.00875500	−0.68767200	−0.00008400
	C2	−1.04271900	0.15278000	0.00006800
	C3	−0.60820500	1.49561500	−0.00001000
	N4	0.72848700	1.49980500	−0.00013900
	C5	1.02289200	0.17449800	0.00021400
	N6	2.39809700	−0.28461200	0.00067900
	O7	3.29154400	0.56477300	−0.00031100
	O8	2.60950000	−1.49786000	−0.00025100
	N9	−2.39909000	−0.30038300	0.00022400
	O10	−3.28335800	0.57377800	−0.00011300
	O11	−2.64065600	−1.50622800	−0.00012600
	H12	−1.20179300	2.39696700	0.00003300

SCF Done: E(B3LYP, cation) = −674.7075741 a.u.

SCF Done: E(B3LYP, anion) = −634.8962734 a.u.

Table S131: Salt 131

Cartesian coordinates

	Atom	X	Y	Z
Cation	O1	−2.41721000	−1.63070300	0.00001300
	N2	−3.21717600	−0.34953200	0.00001200
	C3	−2.31548800	0.62805900	−0.00001500
	C4	−1.03473300	0.00120200	−0.00000200
	N5	−1.12730300	−1.31188400	−0.00003000
	O6	−4.41855900	−0.42314100	0.00002200

	C7	−2.72749400	2.06173600	−0.00003100
	C8	0.25640000	0.67453000	0.00002500
	N9	1.34268400	−0.00020500	0.00000800
	N10	2.52825500	0.68461500	0.00001700
	C11	3.66751000	−0.03976900	−0.00000100
	N12	4.84602300	0.59214800	0.00000500
	N13	3.57842000	−1.36176800	−0.00002100
	H14	−3.81569700	2.12749100	−0.00041800
	H15	−2.35725500	2.58076800	0.88829000
	H16	−2.35660700	2.58092500	−0.88798800
	H17	0.24820400	1.76774100	0.00004600
	H18	2.56191000	1.70080000	0.00003800
	H19	5.71362000	0.07824100	−0.00000200
	H20	4.91099100	1.59823400	0.00001800
	H21	4.39380900	−1.95431400	−0.00003700
	H22	2.65367600	−1.77728600	−0.00002200
Anion	N1	−1.81120700	1.72418200	0.00000000
	N2	−0.79668000	2.57503900	0.00000000
	N3	0.35873200	1.89717100	0.00000000
	C4	0.00000000	0.58544800	0.00000000
	N5	−1.34623900	0.45662100	0.00000000
	N6	1.04723100	−0.34007800	0.00000000
	N7	0.81628700	−1.62454700	0.00000000
	O8	1.85074100	−2.38952400	0.00000000
	O9	−0.33534800	−2.15190100	0.00000000

SCF Done: E(B3LYP, cation) = −674.7075741 a.u.

SCF Done: E(B3LYP, anion) = −517.0427728 a.u.

Table S132: Salt 132

Cartesian coordinates

	Atom	X	Y	Z
Cation	O1	−2.41721000	−1.63070300	0.00001300
	N2	−3.21717600	−0.34953200	0.00001200
	C3	−2.31548800	0.62805900	−0.00001500
	C4	−1.03473300	0.00120200	−0.00000200
	N5	−1.12730300	−1.31188400	−0.00003000
	O6	−4.41855900	−0.42314100	0.00002200
	C7	−2.72749400	2.06173600	−0.00003100
	C8	0.25640000	0.67453000	0.00002500
	N9	1.34268400	−0.00020500	0.00000800
	N10	2.52825500	0.68461500	0.00001700

	C11	3.66751000	−0.03976900	−0.00000100
	N12	4.84602300	0.59214800	0.00000500
	N13	3.57842000	−1.36176800	−0.00002100
	H14	−3.81569700	2.12749100	−0.00041800
	H15	−2.35725500	2.58076800	0.88829000
	H16	−2.35660700	2.58092500	−0.88798800
	H17	0.24820400	1.76774100	0.00004600
	H18	2.56191000	1.70080000	0.00003800
	H19	5.71362000	0.07824100	−0.00000200
	H20	4.91099100	1.59823400	0.00001800
	H21	4.39380900	−1.95431400	−0.00003700
	H22	2.65367600	−1.77728600	−0.00002200
Anion	N1	−3.97109800	−1.75691000	1.87261300
	N2	−2.98430100	−1.03901700	1.33777000
	C3	−3.60589500	−0.19915300	0.49279600
	N4	−4.94010300	−0.37919200	0.48746600
	N5	−5.13769100	−1.36719600	1.35956200
	C6	−2.91663900	0.79966300	−0.30367000
	N7	−3.49857500	1.89095200	−0.74118100
	O8	−2.53466200	2.56555700	−1.48307000
	N9	−1.34649500	1.90459000	−1.48073500
	C10	−1.54382200	0.82814500	−0.76292100
	N11	−0.59307300	−0.20001700	−0.64757200
	N12	0.59309300	0.20049800	−0.64776100
	C13	1.54379900	−0.82777700	−0.76327000
	C14	2.91666100	−0.79952000	−0.30413200
	N15	3.49840900	−1.89089800	−0.74166000
	O16	2.53422700	−2.56539200	−1.48347400
	N17	1.34622000	−1.90424100	−1.48096800
	C18	3.60606800	0.19911300	0.49241600
	N19	4.94048900	0.37781200	0.48864000
	N20	5.13801500	1.36599300	1.36052800
	N21	3.97113100	1.75706800	1.87205000
	N22	2.98432700	1.03996500	1.33625200

SCF Done: E(B3LYP, cation) = −674.7075741 a.u.

SCF Done: E(B3LYP, anion) = −1145.6620709 a.u.

Table S133: Salt 133

Cartesian coordinates

	Atom	X	Y	Z

Cation	C1	1.07570400	0.33131400	0.00000000
	N2	0.00000000	1.09962100	0.00000000
	N3	−1.15290400	0.38196600	0.00000000
	C4	−0.75844100	−0.85881400	0.00000000
	N5	0.61778200	−0.92637500	0.00000000
	H6	2.10682100	0.65010800	0.00000000
	H7	−0.04266000	2.11387400	0.00000000
	H8	−1.40913300	−1.71930500	0.00000000
	H9	1.18725500	−1.76616000	0.00000000
Anion	C1	2.42471400	0.41201200	−0.00007800
	N2	3.23290400	1.47427100	−0.00000900
	O3	2.37576200	2.59302100	−0.00013600
	N4	1.07520000	2.23285000	−0.00028700
	C5	1.06077000	0.92735000	−0.00024600
	C6	−0.23033200	0.26992000	−0.00016200
	N7	−1.39553900	1.02161500	0.00012600
	C8	−2.45817000	0.17025000	0.00013100
	N9	−1.88027000	−1.05122400	−0.00011300
	N10	−0.50899900	−1.00467000	−0.00029600
	N11	2.62885900	−0.92121900	−0.00005700
	N12	3.91426000	−1.35535100	0.00015400
	O13	4.06331500	−2.58771100	0.00006300
	O14	4.87312900	−0.56358600	0.00041300
	N15	−3.70722200	0.63048100	0.00038200
	N16	−4.69342000	−0.30937700	0.00009400
	O17	−5.84329200	0.11397400	0.00035900
	O18	−4.41845100	−1.53194000	−0.00047200
	H19	−1.45036500	2.02949400	0.00066300
	H20	−2.39564200	−1.91837100	−0.00030200

SCF Done: E(B3LYP, cation) = −242.6694056 a.u.

SCF Done: E(B3LYP, anion) = −1022.5658661 a.u.

Table S134: Salt 134

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.00001200	0.00000000	0.00000000
	H2	0.09263200	0.83857300	−0.58434300
	H3	0.10779100	−0.83730900	−0.58355400
	H4	0.72571300	0.00690600	0.72562600
	H5	−0.92605200	−0.00816900	0.44227100
Anion	C1	−2.38294800	0.39604700	−0.01685100

	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −56.9203571 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S135: Salt 135

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.65541700	−0.00411800	0.00005100
	N2	−0.75045600	−0.00232700	−0.00003900
	H3	0.99718400	0.96411800	−0.00012100
	H4	1.05415400	−0.45557600	0.83700000
	H5	1.05425800	−0.45589200	−0.83667700
	H6	−1.21844400	−0.89213100	−0.00011000
	H7	−1.22187800	0.88459500	−0.00017400
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700

	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −112.2418137 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S136: Salt 136

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.62157632	0.00638917	0.00006179
	O2	−0.73539340	0.09712580	−0.00012371
	H3	1.01706940	0.92485812	−0.00007138
	H4	0.92261491	−0.48604256	0.81669314
	H5	0.92281651	−0.48636615	−0.81629998
	H6	−1.11506675	−0.78460439	0.00000414
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −132.0865145 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S137: Salt 137

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800
	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200
	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S138: Salt 138

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.71309600	1.63579100	0.00000000
	C2	0.00000000	0.49075400	0.00000000
	N3	1.34087600	0.55400700	0.00000000
	N4	−0.63397000	−0.66964200	0.00000000
	N5	−0.05044100	−1.92877000	0.00000000
	H6	−1.72036800	1.63935700	0.00000000
	H7	−0.25478500	2.53240900	0.00000000
	H8	1.92947100	−0.26070500	0.00000000
	H9	1.81369600	1.44397200	0.00000000
	H10	−1.64306300	−0.68139000	0.00000000
	H11	−0.67178300	−2.71571000	0.00000000
	H12	0.94325200	−2.04216900	0.00000000
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S139: Salt 139

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.23126100	−0.61392200	−0.00005700
	C2	−0.06944600	0.01029100	−0.00002200
	N3	−2.41564800	0.10939600	−0.00009600

	N4	1.12200500	−0.76734500	0.00008400
	N5	2.24162600	0.08278500	0.00006100
	O6	0.09192400	1.23885400	0.00003400
	H7	−1.31636200	−1.61920200	−0.00004200
	H8	−3.27674900	−0.40124900	−0.00008900
	H9	−2.33833700	1.11046000	−0.00012000
	H10	1.25457300	−1.76698500	0.00002500
	H11	1.70267300	1.03124200	0.00000300
	H12	2.81920300	−0.00159200	0.84339400
	H13	2.81922300	−0.00165200	−0.84325300
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −336.3373235 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S140: Salt 140

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.07570400	0.33131400	0.00000000
	N2	0.00000000	1.09962100	0.00000000
	N3	−1.15290400	0.38196600	0.00000000
	C4	−0.75844100	−0.85881400	0.00000000
	N5	0.61778200	−0.92637500	0.00000000
	H6	2.10682100	0.65010800	0.00000000

	H7	−0.04266000	2.11387400	0.00000000
	H8	−1.40913300	−1.71930500	0.00000000
	H9	1.18725500	−1.76616000	0.00000000
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −242.6694056 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S141: Salt 141

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.08228900	−0.13710400	0.00000000
	N2	−0.61573600	−1.38850300	0.00000000
	N3	0.72573800	−1.43573300	0.00000000
	C4	1.10022700	−0.18529000	0.00000000
	N5	0.00000000	0.65115400	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	−2.11338600	0.17676100	0.00000000
	H8	−1.15210300	−2.24869500	0.00000000
	H9	2.12050200	0.16391300	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900

	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300
	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S142: Salt 142

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.14623600	0.03333100	0.00000000
	N2	−0.77808300	−1.27764000	0.00000000
	C3	0.52291600	−1.45275200	0.00000000
	N4	1.05687000	−0.21481200	0.00000000
	C5	0.00000000	0.68776000	0.00000000
	N6	0.13955500	2.01763800	0.00000000
	H7	−1.49806000	−1.99128000	0.00000000
	H8	1.06053600	−2.38757900	0.00000000
	H9	2.04787200	−0.00691200	0.00000000
	H10	−0.68962500	2.59303300	0.00000000
	H11	1.03703700	2.47307500	0.00000000
Anion	C1	−2.38294800	0.39604700	−0.01685100
	N2	−3.32317700	1.32962300	−0.03254900
	O3	−2.63382800	2.54841200	0.08305200
	N4	−1.27848000	2.35454600	0.17855600
	C5	−1.08980200	1.07043700	0.12410100
	C6	0.27248800	0.51275800	0.20063200
	N7	1.28684600	0.93030500	−0.60510300

	C8	2.34233900	0.22799500	−0.17034900
	N9	1.92983900	−0.56566300	0.85814000
	N10	0.60795400	−0.39556600	1.10898700
	N11	−2.43177200	−0.96073300	−0.15608400
	N12	−3.63060400	−1.54669800	−0.22422100
	O13	−3.62845600	−2.78571600	−0.42360200
	O14	−4.70442300	−0.91500400	−0.08805200
	N15	3.58741400	0.36057000	−0.73404400
	N16	4.57724700	−0.34999700	−0.22622600
	O17	5.70896300	−0.21273000	−0.74683100
	O18	4.42558700	−1.15195700	0.75550100
	H19	2.52792100	−1.20217800	1.36206300

SCF Done: E(B3LYP, cation) = −298.0617301 a.u.

SCF Done: E(B3LYP, anion) = −1021.9625241 a.u.

Table S143: Salt 143

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.00001200	0.00000000	0.00000000
	H2	0.09263200	0.83857300	−0.58434300
	H3	0.10779100	−0.83730900	−0.58355400
	H4	0.72571300	0.00690600	0.72562600
	H5	−0.92605200	−0.00816900	0.44227100
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500
	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100
	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −56.9203571 a.u.
SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S144: Salt 144

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.65541700	−0.00411800	0.00005100
	N2	−0.75045600	−0.00232700	−0.00003900
	H3	0.99718400	0.96411800	−0.00012100
	H4	1.05415400	−0.45557600	0.83700000
	H5	1.05425800	−0.45589200	−0.83667700
	H6	−1.21844400	−0.89213100	−0.00011000
	H7	−1.22187800	0.88459500	−0.00017400
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500
	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100
	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −112.2418137 a.u.
SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S145: Salt 145

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.62157632	0.00638917	0.00006179
	O2	−0.73539340	0.09712580	−0.00012371

	H3	1.01706940	0.92485812	−0.00007138
	H4	0.92261491	−0.48604256	0.81669314
	H5	0.92281651	−0.48636615	−0.81629998
	H6	−1.11506675	−0.78460439	0.00000414
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500
	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100
	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −132.0865145 a.u.

SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S146: Salt 146

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.01505600	1.33482600	−0.00016400
	C2	0.00005600	0.00000600	0.00002800
	N3	1.14853800	−0.68050900	0.00012700
	N4	−1.16365100	−0.65433800	−0.00009900
	H5	0.86148500	1.85114100	−0.18670200
	H6	−0.81953400	1.86956400	0.18784900
	H7	2.02923800	−0.22498500	0.18640200
	H8	1.17252800	−1.67159400	−0.18697800
	H9	−1.20975100	−1.64457800	0.18733500
	H10	−2.03389600	−0.17943500	−0.18712000
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200

N4	2.42720300	−1.94786100	−0.14365200
C5	1.68288300	−0.87493300	−0.03591600
C6	0.23122400	−0.84078900	0.01650100
N7	−0.43311200	0.32435600	−0.16591300
C8	−1.72520800	−0.03870000	−0.06514500
N9	−1.75713900	−1.38974900	0.17040100
N10	−0.51462900	−1.91799900	0.22761700
N11	2.30210000	1.67723600	0.13147700
O12	2.00901300	2.04761300	1.25325100
O13	2.42502300	2.37005200	−0.86162400
N14	−2.74062100	0.85126100	−0.19553800
N15	−3.98632500	0.38456900	−0.07364800
O16	−4.90720200	1.20302900	−0.20020800
O17	−4.23468800	−0.83928700	0.16204000
H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −205.8356358 a.u.

SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S147: Salt 147

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−0.71309600	1.63579100	0.00000000
	C2	0.00000000	0.49075400	0.00000000
	N3	1.34087600	0.55400700	0.00000000
	N4	−0.63397000	−0.66964200	0.00000000
	N5	−0.05044100	−1.92877000	0.00000000
	H6	−1.72036800	1.63935700	0.00000000
	H7	−0.25478500	2.53240900	0.00000000
	H8	1.92947100	−0.26070500	0.00000000
	H9	1.81369600	1.44397200	0.00000000
	H10	−1.64306300	−0.68139000	0.00000000
	H11	−0.67178300	−2.71571000	0.00000000
	H12	0.94325200	−2.04216900	0.00000000
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500

	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100
	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −261.143769 a.u.

SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S148: Salt 148

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	−1.23126100	−0.61392200	−0.00005700
	C2	−0.06944600	0.01029100	−0.00002200
	N3	−2.41564800	0.10939600	−0.00009600
	N4	1.12200500	−0.76734500	0.00008400
	N5	2.24162600	0.08278500	0.00006100
	O6	0.09192400	1.23885400	0.00003400
	H7	−1.31636200	−1.61920200	−0.00004200
	H8	−3.27674900	−0.40124900	−0.00008900
	H9	−2.33833700	1.11046000	−0.00012000
	H10	1.25457300	−1.76698500	0.00002500
	H11	1.70267300	1.03124200	0.00000300
	H12	2.81920300	−0.00159200	0.84339400
	H13	2.81922300	−0.00165200	−0.84325300
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500
	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100

	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −336.3373235 a.u.

SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S149: Salt 149

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	1.07570400	0.33131400	0.00000000
	N2	0.00000000	1.09962100	0.00000000
	N3	−1.15290400	0.38196600	0.00000000
	C4	−0.75844100	−0.85881400	0.00000000
	N5	0.61778200	−0.92637500	0.00000000
	H6	2.10682100	0.65010800	0.00000000
	H7	−0.04266000	2.11387400	0.00000000
	H8	−1.40913300	−1.71930500	0.00000000
	H9	1.18725500	−1.76616000	0.00000000
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500
	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100
	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −242.6694056 a.u.

SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S150: Salt 150

Cartesian coordinates

	Atom	X	Y	Z
Cation	C1	−1.08228900	−0.13710400	0.00000000
	N2	−0.61573600	−1.38850300	0.00000000
	N3	0.72573800	−1.43573300	0.00000000
	C4	1.10022700	−0.18529000	0.00000000
	N5	0.00000000	0.65115400	0.00000000
	N6	0.02662600	2.01061000	0.00000000
	H7	−2.11338600	0.17676100	0.00000000
	H8	−1.15210300	−2.24869500	0.00000000
	H9	2.12050200	0.16391300	0.00000000
	H10	0.92340300	2.46433500	0.00000000
	H11	−0.84244300	2.51536000	0.00000000
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500
	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100
	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −297.9953294 a.u.

SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S151: Salt 151

Cartesian coordinates

	Atom	X	Y	Z

Cation	N1	−1.14623600	0.03333100	0.00000000
	N2	−0.77808300	−1.27764000	0.00000000
	C3	0.52291600	−1.45275200	0.00000000
	N4	1.05687000	−0.21481200	0.00000000
	C5	0.00000000	0.68776000	0.00000000
	N6	0.13955500	2.01763800	0.00000000
	H7	−1.49806000	−1.99128000	0.00000000
	H8	1.06053600	−2.38757900	0.00000000
	H9	2.04787200	−0.00691200	0.00000000
	H10	−0.68962500	2.59303300	0.00000000
	H11	1.03703700	2.47307500	0.00000000
Anion	C1	2.58189000	0.24147100	−0.01939400
	N2	3.81210100	−0.14870400	−0.10559200
	O3	3.73524400	−1.51122400	−0.17745200
	N4	2.42720300	−1.94786100	−0.14365200
	C5	1.68288300	−0.87493300	−0.03591600
	C6	0.23122400	−0.84078900	0.01650100
	N7	−0.43311200	0.32435600	−0.16591300
	C8	−1.72520800	−0.03870000	−0.06514500
	N9	−1.75713900	−1.38974900	0.17040100
	N10	−0.51462900	−1.91799900	0.22761700
	N11	2.30210000	1.67723600	0.13147700
	O12	2.00901300	2.04761300	1.25325100
	O13	2.42502300	2.37005200	−0.86162400
	N14	−2.74062100	0.85126100	−0.19553800
	N15	−3.98632500	0.38456900	−0.07364800
	O16	−4.90720200	1.20302900	−0.20020800
	O17	−4.23468800	−0.83928700	0.16204000
	H18	−2.61090500	−1.91550400	0.29959600

SCF Done: E(B3LYP, cation) = −298.0617301 a.u.

SCF Done: E(B3LYP, anion) = −967.2011174 a.u.

Table S152: Salt 152

Cartesian coordinates

	Atom	X	Y	Z
Cation	N1	0.65541700	−0.00411800	0.00005100
	N2	−0.75045600	−0.00232700	−0.00003900
	H3	0.99718400	0.96411800	−0.00012100
	H4	1.05415400	−0.45557600	0.83700000
	H5	1.05425800	−0.45589200	−0.83667700
	H6	−1.21844400	−0.89213100	−0.00011000

	H7	−1.22187800	0.88459500	−0.00017400
Anion	C1	0.00000000	0.00000000	0.00000000
	N2	0.00000000	1.44647000	0.00000000
	O3	1.07697200	2.05098400	0.00000000
	O4	−1.07697200	2.05098400	0.00000000
	N5	−1.25268000	−0.72323500	0.00000000
	O6	−1.23771800	−1.95817700	0.00000000
	O7	−2.31469000	−0.09280700	0.00000000
	N8	1.25268000	−0.72323500	0.00000000
	O9	1.23771800	−1.95817700	0.00000000
	O10	2.31469000	−0.09280700	0.00000000

SCF Done: E(B3LYP, cation) = −112.2418137 a.u.

SCF Done: E(B3LYP, anion) = −653.654036 a.u.