FOUNDATIONS

ADVANCES

Volume 79 (2023)

Supporting information for article:

Revisited relativistic Dirac–Hartree–Fock X-ray scattering factors. II. Chemically relevant cations and selected monovalent anions for atoms with *Z* = 2–112

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Table S1. Electron configurations of the calculated species in the ground state. The symbol in the square brackets represents the core electron configuration of a noble gas in the preceding period.

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
1	Li(1+)	1s(2)	1s(2)	———
2	Be(2+)	1s(2)	1s(2)	———
3	B(1+)	[He] 2s(2)	[He] 2s(2)	[He] 2s(2)
4	B(2+)	[He] 2s(1)	[He] 2s(1)	[He] 2s(1)
5	B(3+)	1s(2)	1s(2)	1s(2)
6	C(1+)	[He] 2s(2) 2p(1)	[He] 2s(2) 2p(1)	[He] 2s(2) 2p(1)
7	C(2+)	[He] 2s(2)	[He] 2s(2)	[He] 2s(2)
8	C(3+)	[He] 2s(1)	[He] 2s(1)	[He] 2s(1)
9	C(4+)	1s(2)	1s(2)	1s(2)
10	C(val)	[He] 2s(1) 2p(3)	———	———
11	N(1+)	[He] 2s(2) 2p(2)	[He] 2s(2) 2p(2)	[He] 2s(2) 2p(2)
12	N(2+)	[He] 2s(2) 2p(1)	[He] 2s(2) 2p(1)	[He] 2s(2) 2p(1)
13	N(3+)	[He] 2s(2)	[He] 2s(2)	[He] 2s(2)
14	N(4+)	[He] 2s(1)	[He] 2s(1)	[He] 2s(1)
15	N(5+)	1s(2)	1s(2)	1s(2)
16	O(1+)	[He] 2s(2) 2p(3)	[He] 2s(2) 2p(3)	[He] 2s(2) 2p(3)
17	O(2+)	[He] 2s(2) 2p(2)	[He] 2s(2) 2p(2)	[He] 2s(2) 2p(2)
18	O(1-)	[He] 2s(2) 2p(5)	———	———
19	F(1-)	[He] 2s(2) 2p(6)	———	———
20	Na(1+)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)
21	Mg(2+)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)
22	Al(1+)	[Ne] 3s(2)	[Ne] 3s(2)	[Ne] 3s(2)
23	Al(3+)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)
24	Si(1+)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)
25	Si(2+)	[Ne] 3s(2)	[Ne] 3s(2)	[Ne] 3s(2)
26	Si(3+)	[Ne] 3s(1)	[Ne] 3s(1)	[Ne] 3s(1)
27	Si(4+)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)
28	Si(val)	[Ne] 3s(1) 3p(3)	———	———
29	P(1+)	[Ne] 3s(2) 3p(2)	[Ne] 3s(2) 3p(2)	[Ne] 3s(2) 3p(2)
30	P(2+)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)
31	P(3+)	[Ne] 3s(2)	[Ne] 3s(2)	[Ne] 3s(2)
32	P(4+)	[Ne] 3s(1)	[Ne] 3s(1)	[Ne] 3s(1)
33	P(5+)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)
34	S(1+)	[Ne] 3s(2) 3p(3)	[Ne] 3s(2) 3p(3)	[Ne] 3s(2) 3p(3)
35	S(2+)	[Ne] 3s(2) 3p(2)	[Ne] 3s(2) 3p(2)	[Ne] 3s(2) 3p(2)
36	S(3+)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)
37	S(4+)	[Ne] 3s(2)	[Ne] 3s(2)	[Ne] 3s(2)
38	S(5+)	[Ne] 3s(1)	[Ne] 3s(1)	[Ne] 3s(1)
39	S(6+)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)

| 40 | Cl(1+) | [Ne] 3s(2) 3p(4) | [Ne] 3s(2) 3p(4) | [Ne] 3s(2) 3p(4) |

Table S1 (continued).

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
41	Cl(2+)	[Ne] 3s(2) 3p(3)	[Ne] 3s(2) 3p(3)	[Ne] 3s(2) 3p(3)
42	Cl(3+)	[Ne] 3s(2) 3p(2)	[Ne] 3s(2) 3p(2)	[Ne] 3s(2) 3p(2)
43	Cl(4+)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)	[Ne] 3s(2) 3p(1)
44	Cl(5+)	[Ne] 3s(2)	[Ne] 3s(2)	[Ne] 3s(2)
45	Cl(6+)	[Ne] 3s(1)	[Ne] 3s(1)	[Ne] 3s(1)
46	Cl(7+)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)	[He] 2s(2) 2p(6)
47	Cl(1-)	[Ne] 3s(2) 3p(6)	———	———
48	K(1+)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)
49	Ca(2+)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)
50	Sc(1+)	[Ar] 3d(1) 4s(1)	[Ar] 3d(1) 4s(1)	[Ar] 3d(1) 4s(1)
51	Sc(2+)	[Ar] 3d(1)	[Ar] 3d(1)	[Ar] 3d(1)
52	Sc(3+)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)
53	Ti(2+)	[Ar] 3d(2)	[Ar] 3d(2)	[Ar] 3d(2)
54	Ti(3+)	[Ar] 3d(1)	[Ar] 3d(1)	[Ar] 3d(1)
55	Ti(4+)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)
56	V(1+)	[Ar] 3d(4)	[Ar] 3d(4)	[Ar] 3d(4)
57	V(2+)	[Ar] 3d(3)	[Ar] 3d(3)	[Ar] 3d(3)
58	V(3+)	[Ar] 3d(2)	[Ar] 3d(2)	[Ar] 3d(2)
59	V(4+)	[Ar] 3d(1)	[Ar] 3d(1)	[Ar] 3d(1)
60	V(5+)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)
61	Cr(1+)	[Ar] 3d(5)	[Ar] 3d(5)	[Ar] 3d(5)
62	Cr(2+)	[Ar] 3d(4)	[Ar] 3d(4)	[Ar] 3d(4)
63	Cr(3+)	[Ar] 3d(3)	[Ar] 3d(3)	[Ar] 3d(3)
64	Cr(4+)	[Ar] 3d(2)	[Ar] 3d(2)	[Ar] 3d(2)
65	Cr(5+)	[Ar] 3d(1)	[Ar] 3d(1)	[Ar] 3d(1)
66	Cr(6+)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)
67	Mn(1+)	[Ar] 3d(5) 4s(1)	[Ar] 3d(5) 4s(1)	[Ar] 3d(5) 4s(1)
68	Mn(2+)	[Ar] 3d(5)	[Ar] 3d(5)	[Ar] 3d(5)
69	Mn(3+)	[Ar] 3d(4)	[Ar] 3d(4)	[Ar] 3d(4)
70	Mn(4+)	[Ar] 3d(3)	[Ar] 3d(3)	[Ar] 3d(3)
71	Mn(5+)	[Ar] 3d(2)	[Ar] 3d(2)	[Ar] 3d(2)
72	Mn(6+)	[Ar] 3d(1)	[Ar] 3d(1)	[Ar] 3d(1)
73	Mn(7+)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)	[Ne] 3s(2) 3p(6)
74	Fe(1+)	[Ar] 3d(6) 4s(1)	[Ar] 3d(6) 4s(1)	[Ar] 3d(6) 4s(1)
75	Fe(2+)	[Ar] 3d(6)	[Ar] 3d(6)	[Ar] 3d(6)
76	Fe(3+)	[Ar] 3d(5)	[Ar] 3d(5)	[Ar] 3d(5)
77	Fe(4+)	[Ar] 3d(4)	[Ar] 3d(4)	[Ar] 3d(4)
78	Fe(5+)	[Ar] 3d(3)	[Ar] 3d(3)	[Ar] 3d(3)
79	Fe(6+)	[Ar] 3d(2)	[Ar] 3d(2)	[Ar] 3d(2)
80	Co(1+)	[Ar] 3d(8)	[Ar] 3d(8)	[Ar] 3d(8)

Table S1 (continued).

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
81	Co(2+)	[Ar] 3d(7)	[Ar] 3d(7)	[Ar] 3d(7)
82	Co(3+)	[Ar] 3d(6)	[Ar] 3d(6)	[Ar] 3d(6)
83	Co(4+)	[Ar] 3d(5)	[Ar] 3d(5)	[Ar] 3d(5)
84	Co(5+)	[Ar] 3d(4)	[Ar] 3d(4)	[Ar] 3d(4)
85	Ni(1+)	[Ar] 3d(9)	[Ar] 3d(9)	[Ar] 3d(9)
86	Ni(2+)	[Ar] 3d(8)	[Ar] 3d(8)	[Ar] 3d(8)
87	Ni(3+)	[Ar] 3d(7)	[Ar] 3d(7)	[Ar] 3d(7)
88	Ni(4+)	[Ar] 3d(6)	[Ar] 3d(6)	[Ar] 3d(6)
89	Cu(1+)	[Ar] 3d(10)	[Ar] 3d(10)	[Ar] 3d(10)
90	Cu(2+)	[Ar] 3d(9)	[Ar] 3d(9)	[Ar] 3d(9)
91	Cu(3+)	[Ar] 3d(8)	[Ar] 3d(8)	[Ar] 3d(8)
92	Cu(4+)	[Ar] 3d(7)	[Ar] 3d(7)	[Ar] 3d(7)
93	Zn(2+)	[Ar] 3d(10)	[Ar] 3d(10)	[Ar] 3d(10)
94	Ga(1+)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)
95	Ga(2+)	[Ar] 3d(10) 4s(1)	[Ar] 3d(10) 4s(1)	[Ar] 3d(10) 4s(1)
96	Ga(3+)	[Ar] 3d(10)	[Ar] 3d(10)	[Ar] 3d(10)
97	Ge(1+)	[Ar] 3d(10) 4s(2) 4p(1)	[Ar] 3d(10) 4s(2) 4p(1)	[Ar] 3d(10) 4s(2) 4p(1)
98	Ge(2+)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)
99	Ge(3+)	[Ar] 3d(10) 4s(1)	[Ar] 3d(10) 4s(1)	[Ar] 3d(10) 4s(1)
100	Ge(4+)	[Ar] 3d(10)	[Ar] 3d(10)	[Ar] 3d(10)
101	As(2+)	[Ar] 3d(10) 4s(2) 4p(1)	[Ar] 3d(10) 4s(2) 4p(1)	[Ar] 3d(10) 4s(2) 4p(1)
102	As(3+)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)
103	As(5+)	[Ar] 3d(10)	[Ar] 3d(10)	[Ar] 3d(10)
104	Se(2+)	[Ar] 3d(10) 4s(2) 4p(2)	[Ar] 3d(10) 4s(2) 4p(2)	[Ar] 3d(10) 4s(2) 4p(2)
105	Se(4+)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)
106	Se(6+)	[Ar] 3d(10)	[Ar] 3d(10)	[Ar] 3d(10)
107	Br(1+)	[Ar] 3d(10) 4s(2) 4p(4)	[Ar] 3d(10) 4s(2) 4p(4)	[Ar] 3d(10) 4s(2) 4p(4)
108	Br(3+)	[Ar] 3d(10) 4s(2) 4p(2)	[Ar] 3d(10) 4s(2) 4p(2)	[Ar] 3d(10) 4s(2) 4p(2)
109	Br(4+)	[Ar] 3d(10) 4s(2) 4p(1)	[Ar] 3d(10) 4s(2) 4p(1)	[Ar] 3d(10) 4s(2) 4p(1)
110	Br(5+)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)	[Ar] 3d(10) 4s(2)
111	Br(7+)	[Ar] 3d(10)	[Ar] 3d(10)	[Ar] 3d(10)
112	Br(1-)	[Ar] 3d(10) 4s(2) 4p(6)	———	———
113	Kr(2+)	[Ar] 3d(10) 4s(2) 4p(4)	[Ar] 3d(10) 4s(2) 4p(4)	[Ar] 3d(10) 4s(2) 4p(4)
114	Rb(1+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
115	Sr(2+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
116	Y(2+)	[Kr] 4d(1)	[Kr] 4d(1)	[Kr] 4d(1)
117	Y(3+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
118	Zr(1+)	[Kr] 4d(2) 5s(1)	[Kr] 4d(2) 5s(1)	[Kr] 4d(2) 5s(1)
119	Zr(2+)	[Kr] 4d(2)	[Kr] 4d(2)	[Kr] 4d(2)
120	Zr(3+)	[Kr] 4d(1)	[Kr] 4d(1)	[Kr] 4d(1)

Table S1 (continued).

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
121	Zr(4+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
122	Nb(2+)	[Kr] 4d(3)	[Kr] 4d(3)	[Kr] 4d(3)
123	Nb(3+)	[Kr] 4d(2)	[Kr] 4d(2)	[Kr] 4d(2)
124	Nb(4+)	[Kr] 4d(1)	[Kr] 4d(1)	[Kr] 4d(1)
125	Nb(5+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
126	Mo(1+)	[Kr] 4d(5)	[Kr] 4d(5)	[Kr] 4d(5)
127	Mo(2+)	[Kr] 4d(4)	[Kr] 4d(4)	[Kr] 4d(4)
128	Mo(3+)	[Kr] 4d(3)	[Kr] 4d(3)	[Kr] 4d(3)
129	Mo(4+)	[Kr] 4d(2)	[Kr] 4d(2)	[Kr] 4d(2)
130	Mo(5+)	[Kr] 4d(1)	[Kr] 4d(1)	[Kr] 4d(1)
131	Mo(6+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
132	Tc(1+)	[Kr] 4d(5) 5s(1)	[Kr] 4d(5) 5s(1)	[Kr] 4d(5) 5s(1)
133	Tc(2+)	[Kr] 4d(5)	[Kr] 4d(5)	[Kr] 4d(5)
134	Tc(3+)	[Kr] 4d(4)	[Kr] 4d(4)	[Kr] 4d(4)
135	Tc(4+)	[Kr] 4d(3)	[Kr] 4d(3)	[Kr] 4d(3)
136	Tc(5+)	[Kr] 4d(2)	[Kr] 4d(2)	[Kr] 4d(2)
137	Tc(6+)	[Kr] 4d(1)	[Kr] 4d(1)	[Kr] 4d(1)
138	Tc(7+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
139	Ru(1+)	[Kr] 4d(7)	[Kr] 4d(7)	[Kr] 4d(7)
140	Ru(2+)	[Kr] 4d(6)	[Kr] 4d(6)	[Kr] 4d(6)
141	Ru(3+)	[Kr] 4d(5)	[Kr] 4d(5)	[Kr] 4d(5)
142	Ru(4+)	[Kr] 4d(4)	[Kr] 4d(4)	[Kr] 4d(4)
143	Ru(5+)	[Kr] 4d(3)	[Kr] 4d(3)	[Kr] 4d(3)
144	Ru(6+)	[Kr] 4d(2)	[Kr] 4d(2)	[Kr] 4d(2)
145	Ru(7+)	[Kr] 4d(1)	[Kr] 4d(1)	[Kr] 4d(1)
146	Ru(8+)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)	[Ar] 3d(10) 4s(2) 4p(6)
147	Rh(1+)	[Kr] 4d(8)	[Kr] 4d(8)	[Kr] 4d(8)
148	Rh(2+)	[Kr] 4d(7)	[Kr] 4d(7)	[Kr] 4d(7)
149	Rh(3+)	[Kr] 4d(6)	[Kr] 4d(6)	[Kr] 4d(6)
150	Rh(4+)	[Kr] 4d(5)	[Kr] 4d(5)	[Kr] 4d(5)
151	Rh(5+)	[Kr] 4d(4)	[Kr] 4d(4)	[Kr] 4d(4)
152	Rh(6+)	[Kr] 4d(3)	[Kr] 4d(3)	[Kr] 4d(3)
153	Pd(2+)	[Kr] 4d(8)	[Kr] 4d(8)	[Kr] 4d(8)
154	Pd(4+)	[Kr] 4d(6)	[Kr] 4d(6)	[Kr] 4d(6)
155	Ag(1+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
156	Ag(2+)	[Kr] 4d(9)	[Kr] 4d(9)	[Kr] 4d(9)
157	Ag(3+)	[Kr] 4d(8)	[Kr] 4d(8)	[Kr] 4d(8)
158	Cd(2+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
159	In(1+)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)
160	In(2+)	[Kr] 4d(10) 5s(1)	[Kr] 4d(10) 5s(1)	[Kr] 4d(10) 5s(1)

Table S1 (continued).

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
161	In(3+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
162	Sn(2+)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)
163	Sn(4+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
164	Sb(3+)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)
165	Sb(5+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
166	Te(2+)	[Kr] 4d(10) 5s(2) 5p(2)	[Kr] 4d(10) 5s(2) 5p(2)	[Kr] 4d(10) 5s(2) 5p(2)
167	Te(4+)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)
168	Te(5+)	[Kr] 4d(10) 5s(1)	[Kr] 4d(10) 5s(1)	[Kr] 4d(10) 5s(1)
169	Te(6+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
170	I(1+)	[Kr] 4d(10) 5s(2) 5p(4)	[Kr] 4d(10) 5s(2) 5p(4)	[Kr] 4d(10) 5s(2) 5p(4)
171	I(3+)	[Kr] 4d(10) 5s(2) 5p(2)	[Kr] 4d(10) 5s(2) 5p(2)	[Kr] 4d(10) 5s(2) 5p(2)
172	I(5+)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)
173	I(7+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
174	I(1-)	[Kr] 4d(10) 5s(2) 5p(6)	———	———
175	Xe(2+)	[Kr] 4d(10) 5s(2) 5p(4)	[Kr] 4d(10) 5s(2) 5p(4)	[Kr] 4d(10) 5s(2) 5p(4)
176	Xe(4+)	[Kr] 4d(10) 5s(2) 5p(2)	[Kr] 4d(10) 5s(2) 5p(2)	[Kr] 4d(10) 5s(2) 5p(2)
177	Xe(6+)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)	[Kr] 4d(10) 5s(2)
178	Xe(8+)	[Kr] 4d(10)	[Kr] 4d(10)	[Kr] 4d(10)
179	Cs(1+)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)
180	Ba(2+)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)
181	La(2+)	[Xe] 5d(1)	[Xe] 5d(1)	[Xe] 5d(1)
182	La(3+)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)
183	Ce(2+)	[Xe] 4f(2)	[Xe] 4f(2)	[Xe] 4f(2)
184	Ce(3+)	[Xe] 4f(1)	[Xe] 4f(1)	[Xe] 4f(1)
185	Ce(4+)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)	[Kr] 4d(10) 5s(2) 5p(6)
186	Pr(2+)	[Xe] 4f(3)	[Xe] 4f(3)	[Xe] 4f(3)
187	Pr(3+)	[Xe] 4f(2)	[Xe] 4f(2)	[Xe] 4f(2)
188	Pr(4+)	[Xe] 4f(1)	[Xe] 4f(1)	[Xe] 4f(1)
189	Nd(2+)	[Xe] 4f(4)	[Xe] 4f(4)	[Xe] 4f(4)
190	Nd(3+)	[Xe] 4f(3)	[Xe] 4f(3)	[Xe] 4f(3)
191	Pm(3+)	[Xe] 4f(4)	[Xe] 4f(4)	[Xe] 4f(4)
192	Sm(2+)	[Xe] 4f(6)	[Xe] 4f(6)	[Xe] 4f(6)
193	Sm(3+)	[Xe] 4f(5)	[Xe] 4f(5)	[Xe] 4f(5)
194	Eu(2+)	[Xe] 4f(7)	[Xe] 4f(7)	[Xe] 4f(7)
195	Eu(3+)	[Xe] 4f(6)	[Xe] 4f(6)	[Xe] 4f(6)
196	Gd(1+)	[Xe] 4f(7) 5d(1) 6s(1)	[Xe] 4f(7) 5d(1) 6s(1)	[Xe] 4f(7) 5d(1) 6s(1)
197	Gd(2+)	[Xe] 4f(7) 5d(1)	[Xe] 4f(7) 5d(1)	[Xe] 4f(7) 5d(1)
198	Gd(3+)	[Xe] 4f(7)	[Xe] 4f(7)	[Xe] 4f(7)
199	Tb(1+)	[Xe] 4f(9) 6s(1)	[Xe] 4f(9) 6s(1)	[Xe] 4f(9) 6s(1)
200	Tb(3+)	[Xe] 4f(8)	[Xe] 4f(8)	[Xe] 4f(8)

Table S1 (continued).

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
201	Tb(4+)	[Xe] 4f(7)	[Xe] 4f(7)	[Xe] 4f(7)
202	Dy(2+)	[Xe] 4f(10)	[Xe] 4f(10)	[Xe] 4f(10)
203	Dy(3+)	[Xe] 4f(9)	[Xe] 4f(9)	[Xe] 4f(9)
204	Ho(3+)	[Xe] 4f(10)	[Xe] 4f(10)	[Xe] 4f(10)
205	Er(3+)	[Xe] 4f(11)	[Xe] 4f(11)	[Xe] 4f(11)
206	Tm(2+)	[Xe] 4f(13)	[Xe] 4f(13)	[Xe] 4f(13)
207	Tm(3+)	[Xe] 4f(12)	[Xe] 4f(12)	[Xe] 4f(12)
208	Yb(2+)	[Xe] 4f(14)	[Xe] 4f(14)	[Xe] 4f(14)
209	Yb(3+)	[Xe] 4f(13)	[Xe] 4f(13)	[Xe] 4f(13)
210	Lu(3+)	[Xe] 4f(14)	[Xe] 4f(14)	[Xe] 4f(14)
211	Hf(2+)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)
212	Hf(3+)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)
213	Hf(4+)	[Xe] 4f(14)	[Xe] 4f(14)	[Xe] 4f(14)
214	Ta(2+)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)
215	Ta(3+)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)
216	Ta(4+)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)
217	Ta(5+)	[Xe] 4f(14)	[Xe] 4f(14)	[Xe] 4f(14)
218	W(1+)	[Xe] 4f(14) 5d(4) 6s(1)	[Xe] 4f(14) 5d(4) 6s(1)	[Xe] 4f(14) 5d(4) 6s(1)
219	W(2+)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)
220	W(3+)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)
221	W(4+)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)
222	W(5+)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)
223	W(6+)	[Xe] 4f(14)	[Xe] 4f(14)	[Xe] 4f(14)
224	Re(1+)	[Xe] 4f(14) 5d(5) 6s(1)	[Xe] 4f(14) 5d(5) 6s(1)	[Xe] 4f(14) 5d(5) 6s(1)
225	Re(2+)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)
226	Re(3+)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)
227	Re(4+)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)
228	Re(5+)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)
229	Re(6+)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)
230	Re(7+)	[Xe] 4f(14)	[Xe] 4f(14)	[Xe] 4f(14)
231	Os(1+)	[Xe] 4f(14) 5d(6) 6s(1)	[Xe] 4f(14) 5d(6) 6s(1)	[Xe] 4f(14) 5d(6) 6s(1)
232	Os(2+)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(5) 6s(1)
233	Os(3+)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)
234	Os(4+)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)
235	Os(5+)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)
236	Os(6+)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)	[Xe] 4f(14) 5d(2)
237	Os(7+)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)	[Xe] 4f(14) 5d(1)
238	Os(8+)	[Xe] 4f(14)	[Xe] 4f(14)	[Xe] 4f(14)
239	Ir(1+)	[Xe] 4f(14) 5d(7) 6s(1)	[Xe] 4f(14) 5d(7) 6s(1)	[Xe] 4f(14) 5d(7) 6s(1)
240	Ir(2+)	[Xe] 4f(14) 5d(7)	[Xe] 4f(14) 5d(7)	[Xe] 4f(14) 5d(7)

Table S1 (continued).

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
241	Ir(3+)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(6)
242	Ir(4+)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)
243	Ir(5+)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)
244	Ir(6+)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)	[Xe] 4f(14) 5d(3)
245	Pt(2+)	[Xe] 4f(14) 5d(8)	[Xe] 4f(14) 5d(8)	[Xe] 4f(14) 5d(8)
246	Pt(4+)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(6)
247	Pt(5+)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)	[Xe] 4f(14) 5d(5)
248	Pt(6+)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)	[Xe] 4f(14) 5d(4)
249	Au(1+)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)
250	Au(2+)	[Xe] 4f(14) 5d(9)	[Xe] 4f(14) 5d(9)	[Xe] 4f(14) 5d(9)
251	Au(3+)	[Xe] 4f(14) 5d(8)	[Xe] 4f(14) 5d(8)	[Xe] 4f(14) 5d(8)
252	Au(5+)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(6)	[Xe] 4f(14) 5d(6)
253	Hg(1+)	[Xe] 4f(14) 5d(10) 6s(1)	[Xe] 4f(14) 5d(10) 6s(1)	[Xe] 4f(14) 5d(10) 6s(1)
254	Hg(2+)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)
255	Tl(1+)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)
256	Tl(3+)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)
257	Pb(2+)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)
258	Pb(4+)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)
259	Bi(3+)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)
260	Bi(5+)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)
261	Po(2+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(2)	[Xe] 4f(14) 5d(10) 6s(2) 6p(2)	[Xe] 4f(14) 5d(10) 6s(2) 6p(2)
262	Po(4+)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)
263	Po(6+)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)
264	At(1+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(4)	[Xe] 4f(14) 5d(10) 6s(2) 6p(4)	[Xe] 4f(14) 5d(10) 6s(2) 6p(4)
265	At(3+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(2)	[Xe] 4f(14) 5d(10) 6s(2) 6p(2)	[Xe] 4f(14) 5d(10) 6s(2) 6p(2)
266	At(5+)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)	[Xe] 4f(14) 5d(10) 6s(2)
267	At(7+)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)	[Xe] 4f(14) 5d(10)
268	At(1-)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	———	———
269	Fr(1+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)
270	Ra(2+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)
271	Ac(3+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)
272	Th(2+)	[Rn] 6d(1) 5f(1)	[Rn] 6d(1) 5f(1)	[Rn] 6d(2)
273	Th(3+)	[Rn] 5f(1)	[Rn] 5f(1)	[Rn] 5f(1)
274	Th(4+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)
275	Pa(3+)	[Rn] 5f(2)	[Rn] 5f(2)	[Rn] 5f(2)
276	Pa(4+)	[Rn] 5f(1)	[Rn] 5f(1)	[Rn] 5f(1)
277	Pa(5+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)
278	U(3+)	[Rn] 5f(3)	[Rn] 5f(3)	[Rn] 5f(3)
279	U(4+)	[Rn] 5f(2)	[Rn] 5f(2)	[Rn] 5f(2)
280	U(5+)	[Rn] 5f(1)	[Rn] 5f(1)	[Rn] 5f(1)

Table S1 (continued).

N.	Ion/Atom	This work	Kramida et al. (2021)	Rodrigues et al. (2004)
281	U(6+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)
282	Np(3+)	[Rn] 5f(4)	[Rn] 5f(4)	[Rn] 5f(4)
283	Np(4+)	[Rn] 5f(3)	[Rn] 5f(3)	[Rn] 5f(3)
284	Np(5+)	[Rn] 5f(2)	[Rn] 5f(2)	[Rn] 5f(2)
285	Np(6+)	[Rn] 5f(1)	[Rn] 5f(1)	[Rn] 5f(1)
286	Np(7+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	[Xe] 4f(14) 5d(10) 6s(2) 6p(5) 5f(1)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)
287	Pu(3+)	[Rn] 5f(5)	[Rn] 5f(5)	[Rn] 5f(5)
288	Pu(4+)	[Rn] 5f(4)	[Rn] 5f(4)	[Rn] 5f(4)
289	Pu(5+)	[Rn] 5f(3)	[Rn] 5f(3)	[Rn] 5f(3)
290	Pu(6+)	[Rn] 5f(2)	[Xe] 4f(14) 5d(10) 6s(2) 6p(5) 5f(3)	[Rn] 5f(2)
291	Pu(7+)	[Rn] 5f(1)	[Xe] 4f(14) 5d(10) 6s(2) 6p(4) 5f(3)	[Rn] 5f(1)
292	Am(2+)	[Rn] 5f(7)	[Rn] 5f(7)	[Rn] 5f(7)
293	Am(3+)	[Rn] 5f(6)	[Rn] 5f(6)	[Rn] 5f(6)
294	Am(4+)	[Rn] 5f(5)	[Rn] 5f(5)	[Rn] 5f(5)
295	Am(5+)	[Rn] 5f(4)	[Rn] 5f(4)	[Rn] 5f(4)
296	Am(6+)	[Rn] 5f(3)	[Rn] 5f(3)	[Rn] 5f(3)
297	Cm(3+)	[Rn] 5f(7)	[Rn] 5f(7)	[Rn] 5f(7)
298	Cm(4+)	[Rn] 5f(6)	[Rn] 5f(6)	[Rn] 5f(6)
299	Bk(3+)	[Rn] 5f(8)	[Rn] 5f(8)	[Rn] 5f(8)
300	Bk(4+)	[Rn] 5f(7)	[Rn] 5f(7)	[Rn] 5f(7)
301	Cf(2+)	[Rn] 5f(10)	[Rn] 5f(10)	[Rn] 5f(10)
302	Cf(3+)	[Rn] 5f(9)	[Rn] 5f(9)	[Rn] 5f(9)
303	Cf(4+)	[Rn] 5f(8)	[Rn] 5f(8)	[Rn] 5f(8)
304	Es(2+)	[Rn] 5f(11)	[Rn] 5f(11)	[Rn] 5f(11)
305	Es(3+)	[Rn] 5f(10)	[Rn] 5f(10)	[Rn] 5f(10)
306	Fm(2+)	[Rn] 5f(12)	[Rn] 5f(12)	[Rn] 5f(12)
307	Fm(3+)	[Rn] 5f(11)	[Rn] 5f(11)	[Rn] 5f(11)
308	Md(2+)	[Rn] 5f(13)	[Rn] 5f(13)	[Rn] 5f(13)
309	Md(3+)	[Rn] 5f(12)	[Rn] 5f(12)	[Rn] 5f(12)
310	No(2+)	[Rn] 5f(14)	[Rn] 5f(14)	[Rn] 5f(14)
311	No(3+)	[Rn] 5f(13)	[Rn] 5f(13)	[Rn] 5f(13)
312	Lr(3+)	[Rn] 5f(14)	[Rn] 5f(14)	[Rn] 5f(14)
313	Rf(4+)	[Rn] 5f(14)	[Rn] 5f(14)	[Rn] 5f(14)
314	Db(5+)	[Rn] 5f(14)	[Rn] 5f(14)	[Rn] 5f(14)
315	Sg(6+)	[Rn] 5f(14)	[Rn] 5f(14)	[Rn] 5f(14)
316	Bh(7+)	[Rn] 5f(14)	[Rn] 5f(14)	[Rn] 5f(14)
317	Hs(8+)	[Rn] 5f(14)	[Rn] 5f(14)	[Rn] 5f(14)
318	Cn(2+)	[Rn] 5f(14) 6d(10)	———	———

Table S2. Electron configuration of neutral atoms in the ground state (labelled as LS) and the generated appropriate relativistic configuration state function (CSFs) with the corresponding weights used in the calculations. For all atoms except helium, the symbol in square brackets represents the core electron configuration of a noble gas in the preceding period. The quantity n(CSF) is the number of configuration state functions for each non-relativistic configuration. DATE = 2022-07-29   TIME = 20:53:12

N.	Z	Atom	LS	n(CSF)		CSF			Weight(CSF)
1	3	Li(1+)	1s(2)	1	:	1s (2)			1.00000
2	4	Be(2+)	1s(2)	1	:	1s (2)			1.00000
3	5	B(1+)	[He] 2s(2)	1	:	2s (2)			1.00000
4	5	B(2+)	[He] 2s(1)	1	:	2s (1)			1.00000
5	5	B(3+)	1s(2)	1	:	1s (2)			1.00000
6	6	C(1+)	[He] 2s(2) 2p(1)	2	:	2s (2)	2p-(1)		0.33333
						2s (2)	2p (1)		0.66667
7	6	C(2+)	[He] 2s(2)	1	:	2s (2)			1.00000
8	6	C(3+)	[He] 2s(1)	1	:	2s (1)			1.00000
9	6	C(4+)	1s(2)	1	:	1s (2)			1.00000
10	6	C(val)	[He] 2s(1) 2p(3)	3	:	2s (1)	2p-(2)	2p (1)	0.20000
						2s (1)	2p-(1)	2p (2)	0.60000
						2s (1)	2p (3)		0.20000
11	7	N(1+)	[He] 2s(2) 2p(2)	3	:	2s (2)	2p-(2)		0.06667
						2s (2)	2p-(1)	2p (1)	0.53333
						2s (2)	2p (2)		0.40000

```
12    7   N(2+)     [He] 2s(2) 2p(1)          2   :   2s ( 2)  2p-( 1)                    0.33333
                                                      2s ( 2)  2p ( 1)                     0.66667


13    7   N(3+)     [He] 2s(2)                1   :   2s ( 2)                              1.00000


14    7   N(4+)     [He] 2s(1)                1   :   2s ( 1)                              1.00000


15    7   N(5+)     1s(2)                     1   :   1s ( 2)                              1.00000


16    8   O(1+)     [He] 2s(2) 2p(3)          3   :   2s ( 2)  2p-( 2)  2p ( 1)           0.20000
                                                      2s ( 2)  2p-( 1)  2p ( 2)           0.60000
                                                      2s ( 2)  2p ( 3)                    0.20000
```

N.	Z	Atom	LS	n(CSF)		CSF			Weight(CSF)
17	8	O(2+)	[He] 2s(2) 2p(2)	3	:	2s (2)	2p-(2)		0.06667
						2s (2)	2p-(1)	2p (1)	0.53333
						2s (2)	2p (2)		0.40000
18	8	O(1-)	[He] 2s(2) 2p(5)	2	:	2s (2)	2p-(2)	2p (3)	0.66667
						2s (2)	2p-(1)	2p (4)	0.33333
19	9	F(1-)	[He] 2s(2) 2p(6)	1	:	2s (2)	2p-(2)	2p (4)	1.00000
20	11	Na(1+)	[He] 2s(2) 2p(6)	1	:	2s (2)	2p-(2)	2p (4)	1.00000
21	12	Mg(2+)	[He] 2s(2) 2p(6)	1	:	2s (2)	2p-(2)	2p (4)	1.00000
22	13	Al(1+)	[Ne] 3s(2)	1	:	3s (2)			1.00000
23	13	Al(3+)	[He] 2s(2) 2p(6)	1	:	2s (2)	2p-(2)	2p (4)	1.00000
24	14	Si(1+)	[Ne] 3s(2) 3p(1)	2	:	3s (2)	3p-(1)		0.33333
						3s (2)	3p (1)		0.66667
25	14	Si(2+)	[Ne] 3s(2)	1	:	3s (2)			1.00000
26	14	Si(3+)	[Ne] 3s(1)	1	:	3s (1)			1.00000
27	14	Si(4+)	[He] 2s(2) 2p(6)	1	:	2s (2)	2p-(2)	2p (4)	1.00000
28	14	Si(val)	[Ne] 3s(1) 3p(3)	3	:	3s (1)	3p-(2)	3p (1)	0.20000
						3s (1)	3p-(1)	3p (2)	0.60000
						3s (1)	3p (3)		0.20000
29	15	P(1+)	[Ne] 3s(2) 3p(2)	3	:	3s (2)	3p-(2)		0.06667
						3s (2)	3p-(1)	3p (1)	0.53333
						3s (2)	3p (2)		0.40000
30	15	P(2+)	[Ne] 3s(2) 3p(1)	2	:	3s (2)	3p-(1)		0.33333

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                                                        3s ( 2)  3p ( 1)                              0.66667

31   15  P(3+)     [Ne] 3s(2)                1   :   3s ( 2)                                          1.00000

32   15  P(4+)     [Ne] 3s(1)                1   :   3s ( 1)                                          1.00000

33   15  P(5+)     [He] 2s(2) 2p(6)          1   :   2s ( 2)  2p-( 2)  2p ( 4)                        1.00000

34   16  S(1+)     [Ne] 3s(2) 3p(3)          3   :   3s ( 2)  3p-( 2)  3p ( 1)                        0.20000
                                                     3s ( 2)  3p-( 1)  3p ( 2)                        0.60000
                                                     3s ( 2)  3p ( 3)                                 0.20000
```

N.	Z	Atom	LS	n(CSF)	CSF			Weight(CSF)
35	16	S(2+)	[Ne] 3s(2) 3p(2)	3 :	3s (2) 3p-(2)			0.06667
					3s (2) 3p-(1)	3p (1)		0.53333
					3s (2) 3p (2)			0.40000
36	16	S(3+)	[Ne] 3s(2) 3p(1)	2 :	3s (2) 3p-(1)			0.33333
					3s (2) 3p (1)			0.66667
37	16	S(4+)	[Ne] 3s(2)	1 :	3s (2)			1.00000
38	16	S(5+)	[Ne] 3s(1)	1 :	3s (1)			1.00000
39	16	S(6+)	[He] 2s(2) 2p(6)	1 :	2s (2) 2p-(2)	2p (4)		1.00000
40	17	Cl(1+)	[Ne] 3s(2) 3p(4)	3 :	3s (2) 3p-(2)	3p (2)		0.40000
					3s (2) 3p-(1)	3p (3)		0.53333
					3s (2) 3p (4)			0.06667
41	17	Cl(2+)	[Ne] 3s(2) 3p(3)	3 :	3s (2) 3p-(2)	3p (1)		0.20000
					3s (2) 3p-(1)	3p (2)		0.60000
					3s (2) 3p (3)			0.20000
42	17	Cl(3+)	[Ne] 3s(2) 3p(2)	3 :	3s (2) 3p-(2)			0.06667
					3s (2) 3p-(1)	3p (1)		0.53333
					3s (2) 3p (2)			0.40000
43	17	Cl(4+)	[Ne] 3s(2) 3p(1)	2 :	3s (2) 3p-(1)			0.33333
					3s (2) 3p (1)			0.66667
44	17	Cl(5+)	[Ne] 3s(2)	1 :	3s (2)			1.00000
45	17	Cl(6+)	[Ne] 3s(1)	1 :	3s (1)			1.00000
46	17	Cl(7+)	[He] 2s(2) 2p(6)	1 :	2s (2) 2p-(2)	2p (4)		1.00000
47	17	Cl(1-)	[Ne] 3s(2) 3p(6)	1 :	3s (2) 3p-(2)	3p (4)		1.00000

48	19	K(1+)	[Ne] 3s(2) 3p(6)	1	:	3s (2)	3p-(2)	3p (4)	1.00000
49	20	Ca(2+)	[Ne] 3s(2) 3p(6)	1	:	3s (2)	3p-(2)	3p (4)	1.00000
50	21	Sc(1+)	[Ar] 3d(1) 4s(1)	2	:	3d-(1)	4s (1)		0.40000
						3d (1)	4s (1)		0.60000
51	21	Sc(2+)	[Ar] 3d(1)	2	:	3d-(1)			0.40000
						3d (1)			0.60000
52	21	Sc(3+)	[Ne] 3s(2) 3p(6)	1	:	3s (2)	3p-(2)	3p (4)	1.00000

N.	Z	Atom	LS	n(CSF)		CSF			Weight(CSF)
53	22	Ti(2+)	[Ar] 3d(2)	3	:	3d-(2)			0.13333
						3d-(1)	3d (1)		0.53333
						3d (2)			0.33333
54	22	Ti(3+)	[Ar] 3d(1)	2	:	3d-(1)			0.40000
						3d (1)			0.60000
55	22	Ti(4+)	[Ne] 3s(2) 3p(6)	1	:	3s (2)	3p-(2)	3p (4)	1.00000
56	23	V(1+)	[Ar] 3d(4)	5	:	3d-(4)			0.00476
						3d-(3)	3d (1)		0.11429
						3d-(2)	3d (2)		0.42857
						3d-(1)	3d (3)		0.38095
						3d (4)			0.07143
57	23	V(2+)	[Ar] 3d(3)	4	:	3d-(3)			0.03333
						3d-(2)	3d (1)		0.30000
						3d-(1)	3d (2)		0.50000
						3d (3)			0.16667
58	23	V(3+)	[Ar] 3d(2)	3	:	3d-(2)			0.13333
						3d-(1)	3d (1)		0.53333
						3d (2)			0.33333
59	23	V(4+)	[Ar] 3d(1)	2	:	3d-(1)			0.40000
						3d (1)			0.60000
60	23	V(5+)	[Ne] 3s(2) 3p(6)	1	:	3s (2)	3p-(2)	3p (4)	1.00000
61	24	Cr(1+)	[Ar] 3d(5)	5	:	3d-(4)	3d (1)		0.02381
						3d-(3)	3d (2)		0.23810
						3d-(2)	3d (3)		0.47619
						3d-(1)	3d (4)		0.23810
						3d (5)			0.02381

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62   24  Cr(2+)    [Ar] 3d(4)                    5   :   3d-( 4)                              0.00476
                                                         3d-( 3)  3d ( 1)                     0.11429
                                                         3d-( 2)  3d ( 2)                     0.42857
                                                         3d-( 1)  3d ( 3)                     0.38095
                                                         3d ( 4)                              0.07143


63   24  Cr(3+)    [Ar] 3d(3)                    4   :   3d-( 3)                              0.03333
                                                         3d-( 2)  3d ( 1)                     0.30000
                                                         3d-( 1)  3d ( 2)                     0.50000
                                                         3d ( 3)                              0.16667
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N.	Z	Atom	LS	n(CSF)		CSF			Weight(CSF)
64	24	Cr(4+)	[Ar] 3d(2)	3	:	3d-(2)			0.13333
						3d-(1)	3d (1)		0.53333
						3d (2)			0.33333
65	24	Cr(5+)	[Ar] 3d(1)	2	:	3d-(1)			0.40000
						3d (1)			0.60000
66	24	Cr(6+)	[Ne] 3s(2) 3p(6)	1	:	3s (2)	3p-(2)	3p (4)	1.00000
67	25	Mn(1+)	[Ar] 3d(5) 4s(1)	5	:	3d-(4)	3d (1)	4s (1)	0.02381
						3d-(3)	3d (2)	4s (1)	0.23810
						3d-(2)	3d (3)	4s (1)	0.47619
						3d-(1)	3d (4)	4s (1)	0.23810
						3d (5)	4s (1)		0.02381
68	25	Mn(2+)	[Ar] 3d(5)	5	:	3d-(4)	3d (1)		0.02381
						3d-(3)	3d (2)		0.23810
						3d-(2)	3d (3)		0.47619
						3d-(1)	3d (4)		0.23810
						3d (5)			0.02381
69	25	Mn(3+)	[Ar] 3d(4)	5	:	3d-(4)			0.00476
						3d-(3)	3d (1)		0.11429
						3d-(2)	3d (2)		0.42857
						3d-(1)	3d (3)		0.38095
						3d (4)			0.07143
70	25	Mn(4+)	[Ar] 3d(3)	4	:	3d-(3)			0.03333
						3d-(2)	3d (1)		0.30000
						3d-(1)	3d (2)		0.50000
						3d (3)			0.16667
71	25	Mn(5+)	[Ar] 3d(2)	3	:	3d-(2)			0.13333
						3d-(1)	3d (1)		0.53333
						3d (2)			0.33333

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72   25  Mn(6+)    [Ar] 3d(1)              2   :   3d-( 1)                              0.40000
                                                   3d ( 1)                              0.60000

73   25  Mn(7+)    [Ne] 3s(2) 3p(6)        1   :   3s ( 2)  3p-( 2)  3p ( 4)            1.00000

74   26  Fe(1+)    [Ar] 3d(6) 4s(1)        5   :   3d-( 4)  3d ( 2)  4s ( 1)            0.07143
                                                   3d-( 3)  3d ( 3)  4s ( 1)            0.38095
                                                   3d-( 2)  3d ( 4)  4s ( 1)            0.42857
                                                   3d-( 1)  3d ( 5)  4s ( 1)            0.11429
                                                   3d ( 6)  4s ( 1)                     0.00476
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N.	Z	Atom	LS	n(CSF)		CSF		Weight(CSF)
75	26	Fe(2+)	[Ar] 3d(6)	5	:	3d-(4)	3d (2)	0.07143
						3d-(3)	3d (3)	0.38095
						3d-(2)	3d (4)	0.42857
						3d-(1)	3d (5)	0.11429
						3d (6)		0.00476
76	26	Fe(3+)	[Ar] 3d(5)	5	:	3d-(4)	3d (1)	0.02381
						3d-(3)	3d (2)	0.23810
						3d-(2)	3d (3)	0.47619
						3d-(1)	3d (4)	0.23810
						3d (5)		0.02381
77	26	Fe(4+)	[Ar] 3d(4)	5	:	3d-(4)		0.00476
						3d-(3)	3d (1)	0.11429
						3d-(2)	3d (2)	0.42857
						3d-(1)	3d (3)	0.38095
						3d (4)		0.07143
78	26	Fe(5+)	[Ar] 3d(3)	4	:	3d-(3)		0.03333
						3d-(2)	3d (1)	0.30000
						3d-(1)	3d (2)	0.50000
						3d (3)		0.16667
79	26	Fe(6+)	[Ar] 3d(2)	3	:	3d-(2)		0.13333
						3d-(1)	3d (1)	0.53333
						3d (2)		0.33333
80	27	Co(1+)	[Ar] 3d(8)	3	:	3d-(4)	3d (4)	0.33333
						3d-(3)	3d (5)	0.53333
						3d-(2)	3d (6)	0.13333
81	27	Co(2+)	[Ar] 3d(7)	4	:	3d-(4)	3d (3)	0.16667
						3d-(3)	3d (4)	0.50000
						3d-(2)	3d (5)	0.30000
						3d-(1)	3d (6)	0.03333

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82   27  Co(3+)    [Ar] 3d(6)                     5   :   3d-( 4)  3d ( 2)                        0.07143
                                                          3d-( 3)  3d ( 3)                        0.38095
                                                          3d-( 2)  3d ( 4)                        0.42857
                                                          3d-( 1)  3d ( 5)                        0.11429
                                                          3d ( 6)                                 0.00476


83   27  Co(4+)    [Ar] 3d(5)                     5   :   3d-( 4)  3d ( 1)                        0.02381
                                                          3d-( 3)  3d ( 2)                        0.23810
                                                          3d-( 2)  3d ( 3)                        0.47619
                                                          3d-( 1)  3d ( 4)                        0.23810
                                                          3d ( 5)                                 0.02381
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N.	Z	Atom	LS	n(CSF)	CSF		Weight(CSF)
84	27	Co(5+)	[Ar] 3d(4)	5 :	3d-(4)		0.00476
					3d-(3)	3d (1)	0.11429
					3d-(2)	3d (2)	0.42857
					3d-(1)	3d (3)	0.38095
					3d (4)		0.07143
85	28	Ni(1+)	[Ar] 3d(9)	2 :	3d-(4)	3d (5)	0.60000
					3d-(3)	3d (6)	0.40000
86	28	Ni(2+)	[Ar] 3d(8)	3 :	3d-(4)	3d (4)	0.33333
					3d-(3)	3d (5)	0.53333
					3d-(2)	3d (6)	0.13333
87	28	Ni(3+)	[Ar] 3d(7)	4 :	3d-(4)	3d (3)	0.16667
					3d-(3)	3d (4)	0.50000
					3d-(2)	3d (5)	0.30000
					3d-(1)	3d (6)	0.03333
88	28	Ni(4+)	[Ar] 3d(6)	5 :	3d-(4)	3d (2)	0.07143
					3d-(3)	3d (3)	0.38095
					3d-(2)	3d (4)	0.42857
					3d-(1)	3d (5)	0.11429
					3d (6)		0.00476
89	29	Cu(1+)	[Ar] 3d(10)	1 :	3d-(4)	3d (6)	1.00000
90	29	Cu(2+)	[Ar] 3d(9)	2 :	3d-(4)	3d (5)	0.60000
					3d-(3)	3d (6)	0.40000
91	29	Cu(3+)	[Ar] 3d(8)	3 :	3d-(4)	3d (4)	0.33333
					3d-(3)	3d (5)	0.53333
					3d-(2)	3d (6)	0.13333
92	29	Cu(4+)	[Ar] 3d(7)	4 :	3d-(4)	3d (3)	0.16667
					3d-(3)	3d (4)	0.50000

						3d-(2) 3d (5)	0.30000
						3d-(1) 3d (6)	0.03333
93	30	Zn(2+)	[Ar] 3d(10)	1	:	3d-(4) 3d (6)	1.00000
94	31	Ga(1+)	[Ar] 3d(10) 4s(2)	1	:	3d-(4) 3d (6) 4s (2)	1.00000
95	31	Ga(2+)	[Ar] 3d(10) 4s(1)	1	:	3d-(4) 3d (6) 4s (1)	1.00000
96	31	Ga(3+)	[Ar] 3d(10)	1	:	3d-(4) 3d (6)	1.00000
97	32	Ge(1+)	[Ar] 3d(10) 4s(2) 4p(1)	2	:	3d-(4) 3d (6) 4s (2) 4p-(1)	0.33333
						3d-(4) 3d (6) 4s (2) 4p (1)	0.66667
98	32	Ge(2+)	[Ar] 3d(10) 4s(2)	1	:	3d-(4) 3d (6) 4s (2)	1.00000
99	32	Ge(3+)	[Ar] 3d(10) 4s(1)	1	:	3d-(4) 3d (6) 4s (1)	1.00000
100	32	Ge(4+)	[Ar] 3d(10)	1	:	3d-(4) 3d (6)	1.00000
101	33	As(2+)	[Ar] 3d(10) 4s(2) 4p(1)	2	:	3d-(4) 3d (6) 4s (2) 4p-(1)	0.33333
						3d-(4) 3d (6) 4s (2) 4p (1)	0.66667
102	33	As(3+)	[Ar] 3d(10) 4s(2)	1	:	3d-(4) 3d (6) 4s (2)	1.00000
103	33	As(5+)	[Ar] 3d(10)	1	:	3d-(4) 3d (6)	1.00000
104	34	Se(2+)	[Ar] 3d(10) 4s(2) 4p(2)	3	:	3d-(4) 3d (6) 4s (2) 4p-(2)	0.06667
						3d-(4) 3d (6) 4s (2) 4p-(1) 4p (1)	0.53333
						3d-(4) 3d (6) 4s (2) 4p (2)	0.40000
105	34	Se(4+)	[Ar] 3d(10) 4s(2)	1	:	3d-(4) 3d (6) 4s (2)	1.00000
106	34	Se(6+)	[Ar] 3d(10)	1	:	3d-(4) 3d (6)	1.00000
107	35	Br(1+)	[Ar] 3d(10) 4s(2) 4p(4)	3	:	3d-(4) 3d (6) 4s (2) 4p-(2) 4p (2)	0.40000
						3d-(4) 3d (6) 4s (2) 4p-(1) 4p (3)	0.53333

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                                                             3d-( 4)   3d ( 6)   4s ( 2)   4p ( 4)                          0.06667

  108   35  Br(3+)    [Ar] 3d(10) 4s(2) 4p(2)        3   :   3d-( 4)   3d ( 6)   4s ( 2)   4p-( 2)                         0.06667
                                                             3d-( 4)   3d ( 6)   4s ( 2)   4p-( 1)   4p ( 1)               0.53333
                                                             3d-( 4)   3d ( 6)   4s ( 2)   4p ( 2)                         0.40000

  109   35  Br(4+)    [Ar] 3d(10) 4s(2) 4p(1)        2   :   3d-( 4)   3d ( 6)   4s ( 2)   4p-( 1)                         0.33333
                                                             3d-( 4)   3d ( 6)   4s ( 2)   4p ( 1)                         0.66667

  110   35  Br(5+)    [Ar] 3d(10) 4s(2)              1   :   3d-( 4)   3d ( 6)   4s ( 2)                                   1.00000

  111   35  Br(7+)    [Ar] 3d(10)                    1   :   3d-( 4)   3d ( 6)                                             1.00000

  112   35  Br(1-)    [Ar] 3d(10) 4s(2) 4p(6)        1   :   3d-( 4)   3d ( 6)   4s ( 2)   4p-( 2)   4p ( 4)               1.00000

  113   36  Kr(2+)    [Ar] 3d(10) 4s(2) 4p(4)        3   :   3d-( 4)   3d ( 6)   4s ( 2)   4p-( 2)   4p ( 2)               0.40000
                                                             3d-( 4)   3d ( 6)   4s ( 2)   4p-( 1)   4p ( 3)               0.53333
                                                             3d-( 4)   3d ( 6)   4s ( 2)   4p ( 4)                         0.06667

  114   37  Rb(1+)    [Ar] 3d(10) 4s(2) 4p(6)        1   :   3d-( 4)   3d ( 6)   4s ( 2)   4p-( 2)   4p ( 4)               1.00000

  115   38  Sr(2+)    [Ar] 3d(10) 4s(2) 4p(6)        1   :   3d-( 4)   3d ( 6)   4s ( 2)   4p-( 2)   4p ( 4)               1.00000

  116   39  Y(2+)     [Kr] 4d(1)                     2   :   4d-( 1)                                                       0.40000
                                                             4d ( 1)                                                      0.60000
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N.	Z	Atom	LS	n(CSF)	CSF	Weight(CSF)
117	39	Y(3+)	[Ar] 3d(10) 4s(2) 4p(6)	1	: 3d-(4) 3d (6) 4s (2) 4p-(2) 4p (4)	1.00000
118	40	Zr(1+)	[Kr] 4d(2) 5s(1)	3	: 4d-(2) 5s (1)	0.13333
					4d-(1) 4d (1) 5s (1)	0.53333
					4d (2) 5s (1)	0.33333
119	40	Zr(2+)	[Kr] 4d(2)	3	: 4d-(2)	0.13333
					4d-(1) 4d (1)	0.53333
					4d (2)	0.33333
120	40	Zr(3+)	[Kr] 4d(1)	2	: 4d-(1)	0.40000
					4d (1)	0.60000
121	40	Zr(4+)	[Ar] 3d(10) 4s(2) 4p(6)	1	: 3d-(4) 3d (6) 4s (2) 4p-(2) 4p (4)	1.00000
122	41	Nb(2+)	[Kr] 4d(3)	4	: 4d-(3)	0.03333
					4d-(2) 4d (1)	0.30000
					4d-(1) 4d (2)	0.50000
					4d (3)	0.16667
123	41	Nb(3+)	[Kr] 4d(2)	3	: 4d-(2)	0.13333
					4d-(1) 4d (1)	0.53333
					4d (2)	0.33333
124	41	Nb(4+)	[Kr] 4d(1)	2	: 4d-(1)	0.40000
					4d (1)	0.60000
125	41	Nb(5+)	[Ar] 3d(10) 4s(2) 4p(6)	1	: 3d-(4) 3d (6) 4s (2) 4p-(2) 4p (4)	1.00000
126	42	Mo(1+)	[Kr] 4d(5)	5	: 4d-(4) 4d (1)	0.02381
					4d-(3) 4d (2)	0.23810
					4d-(2) 4d (3)	0.47619
					4d-(1) 4d (4)	0.23810
					4d (5)	0.02381

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127   42  Mo(2+)    [Kr] 4d(4)                5   :  4d-( 4)                                0.00476
                                                     4d-( 3)  4d ( 1)                        0.11429
                                                     4d-( 2)  4d ( 2)                        0.42857
                                                     4d-( 1)  4d ( 3)                        0.38095
                                                     4d ( 4)                                 0.07143

128   42  Mo(3+)    [Kr] 4d(3)                4   :  4d-( 3)                                0.03333
                                                     4d-( 2)  4d ( 1)                        0.30000
                                                     4d-( 1)  4d ( 2)                        0.50000
                                                     4d ( 3)                                 0.16667
```

N.	Z	Atom	LS	n(CSF)		CSF					Weight(CSF)
129	42	Mo(4+)	[Kr] 4d(2)	3	:	4d-(2)					0.13333
						4d-(1)	4d (1)				0.53333
						4d (2)					0.33333
130	42	Mo(5+)	[Kr] 4d(1)	2	:	4d-(1)					0.40000
						4d (1)					0.60000
131	42	Mo(6+)	[Ar] 3d(10) 4s(2) 4p(6)	1	:	3d-(4)	3d (6)	4s (2)	4p-(2)	4p (4)	1.00000
132	43	Tc(1+)	[Kr] 4d(5) 5s(1)	5	:	4d-(4)	4d (1)	5s (1)			0.02381
						4d-(3)	4d (2)	5s (1)			0.23810
						4d-(2)	4d (3)	5s (1)			0.47619
						4d-(1)	4d (4)	5s (1)			0.23810
						4d (5)	5s (1)				0.02381
133	43	Tc(2+)	[Kr] 4d(5)	5	:	4d-(4)	4d (1)				0.02381
						4d-(3)	4d (2)				0.23810
						4d-(2)	4d (3)				0.47619
						4d-(1)	4d (4)				0.23810
						4d (5)					0.02381
134	43	Tc(3+)	[Kr] 4d(4)	5	:	4d-(4)					0.00476
						4d-(3)	4d (1)				0.11429
						4d-(2)	4d (2)				0.42857
						4d-(1)	4d (3)				0.38095
						4d (4)					0.07143
135	43	Tc(4+)	[Kr] 4d(3)	4	:	4d-(3)					0.03333
						4d-(2)	4d (1)				0.30000
						4d-(1)	4d (2)				0.50000
						4d (3)					0.16667
136	43	Tc(5+)	[Kr] 4d(2)	3	:	4d-(2)					0.13333
						4d-(1)	4d (1)				0.53333
						4d (2)					0.33333

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137   43  Tc(6+)    [Kr] 4d(1)                      2   :   4d-( 1)                                    0.40000
                                                             4d ( 1)                                    0.60000


138   43  Tc(7+)    [Ar] 3d(10) 4s(2) 4p(6)         1   :   3d-( 4)  3d ( 6)  4s ( 2)  4p-( 2)  4p ( 4) 1.00000


139   44  Ru(1+)    [Kr] 4d(7)                      4   :   4d-( 4)  4d ( 3)                            0.16667
                                                             4d-( 3)  4d ( 4)                            0.50000
                                                             4d-( 2)  4d ( 5)                            0.30000
                                                             4d-( 1)  4d ( 6)                            0.03333
```

N.	Z	Atom	LS	n(CSF)		CSF	Weight(CSF)
140	44	Ru(2+)	[Kr] 4d(6)	5	:	4d-(4) 4d (2)	0.07143
						4d-(3) 4d (3)	0.38095
						4d-(2) 4d (4)	0.42857
						4d-(1) 4d (5)	0.11429
						4d (6)	0.00476
141	44	Ru(3+)	[Kr] 4d(5)	5	:	4d-(4) 4d (1)	0.02381
						4d-(3) 4d (2)	0.23810
						4d-(2) 4d (3)	0.47619
						4d-(1) 4d (4)	0.23810
						4d (5)	0.02381
142	44	Ru(4+)	[Kr] 4d(4)	5	:	4d-(4)	0.00476
						4d-(3) 4d (1)	0.11429
						4d-(2) 4d (2)	0.42857
						4d-(1) 4d (3)	0.38095
						4d (4)	0.07143
143	44	Ru(5+)	[Kr] 4d(3)	4	:	4d-(3)	0.03333
						4d-(2) 4d (1)	0.30000
						4d-(1) 4d (2)	0.50000
						4d (3)	0.16667
144	44	Ru(6+)	[Kr] 4d(2)	3	:	4d-(2)	0.13333
						4d-(1) 4d (1)	0.53333
						4d (2)	0.33333
145	44	Ru(7+)	[Kr] 4d(1)	2	:	4d-(1)	0.40000
						4d (1)	0.60000
146	44	Ru(8+)	[Ar] 3d(10) 4s(2) 4p(6)	1	:	3d-(4) 3d (6) 4s (2) 4p-(2) 4p (4)	1.00000
147	45	Rh(1+)	[Kr] 4d(8)	3	:	4d-(4) 4d (4)	0.33333
						4d-(3) 4d (5)	0.53333
						4d-(2) 4d (6)	0.13333

```
148   45  Rh(2+)    [Kr] 4d(7)                    4   :   4d-( 4)  4d ( 3)                    0.16667
                                                          4d-( 3)  4d ( 4)                    0.50000
                                                          4d-( 2)  4d ( 5)                    0.30000
                                                          4d-( 1)  4d ( 6)                    0.03333


149   45  Rh(3+)    [Kr] 4d(6)                    5   :   4d-( 4)  4d ( 2)                    0.07143
                                                          4d-( 3)  4d ( 3)                    0.38095
                                                          4d-( 2)  4d ( 4)                    0.42857
                                                          4d-( 1)  4d ( 5)                    0.11429
                                                          4d ( 6)                             0.00476
```

N.	Z	Atom	LS	n(CSF)		CSF		Weight(CSF)
150	45	Rh(4+)	[Kr] 4d(5)	5	:	4d-(4)	4d (1)	0.02381
						4d-(3)	4d (2)	0.23810
						4d-(2)	4d (3)	0.47619
						4d-(1)	4d (4)	0.23810
						4d (5)		0.02381
151	45	Rh(5+)	[Kr] 4d(4)	5	:	4d-(4)		0.00476
						4d-(3)	4d (1)	0.11429
						4d-(2)	4d (2)	0.42857
						4d-(1)	4d (3)	0.38095
						4d (4)		0.07143
152	45	Rh(6+)	[Kr] 4d(3)	4	:	4d-(3)		0.03333
						4d-(2)	4d (1)	0.30000
						4d-(1)	4d (2)	0.50000
						4d (3)		0.16667
153	46	Pd(2+)	[Kr] 4d(8)	3	:	4d-(4)	4d (4)	0.33333
						4d-(3)	4d (5)	0.53333
						4d-(2)	4d (6)	0.13333
154	46	Pd(4+)	[Kr] 4d(6)	5	:	4d-(4)	4d (2)	0.07143
						4d-(3)	4d (3)	0.38095
						4d-(2)	4d (4)	0.42857
						4d-(1)	4d (5)	0.11429
						4d (6)		0.00476
155	47	Ag(1+)	[Kr] 4d(10)	1	:	4d-(4)	4d (6)	1.00000
156	47	Ag(2+)	[Kr] 4d(9)	2	:	4d-(4)	4d (5)	0.60000
						4d-(3)	4d (6)	0.40000
157	47	Ag(3+)	[Kr] 4d(8)	3	:	4d-(4)	4d (4)	0.33333
						4d-(3)	4d (5)	0.53333
						4d-(2)	4d (6)	0.13333

158	48	Cd(2+)	[Kr] 4d(10)	1	:	4d-(4)	4d (6)		1.00000
159	49	In(1+)	[Kr] 4d(10) 5s(2)	1	:	4d-(4)	4d (6)	5s (2)	1.00000
160	49	In(2+)	[Kr] 4d(10) 5s(1)	1	:	4d-(4)	4d (6)	5s (1)	1.00000
161	49	In(3+)	[Kr] 4d(10)	1	:	4d-(4)	4d (6)		1.00000
162	50	Sn(2+)	[Kr] 4d(10) 5s(2)	1	:	4d-(4)	4d (6)	5s (2)	1.00000
163	50	Sn(4+)	[Kr] 4d(10)	1	:	4d-(4)	4d (6)		1.00000

N.	Z	Atom	LS	n(CSF)		CSF					Weight(CSF)
164	51	Sb(3+)	[Kr] 4d(10) 5s(2)	1	:	4d-(4)	4d (6)	5s (2)			1.00000
165	51	Sb(5+)	[Kr] 4d(10)	1	:	4d-(4)	4d (6)				1.00000
166	52	Te(2+)	[Kr] 4d(10) 5s(2) 5p(2)	3	:	4d-(4)	4d (6)	5s (2)	5p-(2)		0.06667
						4d-(4)	4d (6)	5s (2)	5p-(1)	5p (1)	0.53333
						4d-(4)	4d (6)	5s (2)	5p (2)		0.40000
167	52	Te(4+)	[Kr] 4d(10) 5s(2)	1	:	4d-(4)	4d (6)	5s (2)			1.00000
168	52	Te(5+)	[Kr] 4d(10) 5s(1)	1	:	4d-(4)	4d (6)	5s (1)			1.00000
169	52	Te(6+)	[Kr] 4d(10)	1	:	4d-(4)	4d (6)				1.00000
170	53	I(1+)	[Kr] 4d(10) 5s(2) 5p(4)	3	:	4d-(4)	4d (6)	5s (2)	5p-(2)	5p (2)	0.40000
						4d-(4)	4d (6)	5s (2)	5p-(1)	5p (3)	0.53333
						4d-(4)	4d (6)	5s (2)	5p (4)		0.06667
171	53	I(3+)	[Kr] 4d(10) 5s(2) 5p(2)	3	:	4d-(4)	4d (6)	5s (2)	5p-(2)		0.06667
						4d-(4)	4d (6)	5s (2)	5p-(1)	5p (1)	0.53333
						4d-(4)	4d (6)	5s (2)	5p (2)		0.40000
172	53	I(5+)	[Kr] 4d(10) 5s(2)	1	:	4d-(4)	4d (6)	5s (2)			1.00000
173	53	I(7+)	[Kr] 4d(10)	1	:	4d-(4)	4d (6)				1.00000
174	53	I(1-)	[Kr] 4d(10) 5s(2) 5p(6)	1	:	4d-(4)	4d (6)	5s (2)	5p-(2)	5p (4)	1.00000
175	54	Xe(2+)	[Kr] 4d(10) 5s(2) 5p(4)	3	:	4d-(4)	4d (6)	5s (2)	5p-(2)	5p (2)	0.40000
						4d-(4)	4d (6)	5s (2)	5p-(1)	5p (3)	0.53333
						4d-(4)	4d (6)	5s (2)	5p (4)		0.06667
176	54	Xe(4+)	[Kr] 4d(10) 5s(2) 5p(2)	3	:	4d-(4)	4d (6)	5s (2)	5p-(2)		0.06667
						4d-(4)	4d (6)	5s (2)	5p-(1)	5p (1)	0.53333
						4d-(4)	4d (6)	5s (2)	5p (2)		0.40000

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177   54   Xe(6+)     [Kr] 4d(10) 5s(2)              1   :   4d-( 4)  4d ( 6)  5s ( 2)                          1.00000

178   54   Xe(8+)     [Kr] 4d(10)                    1   :   4d-( 4)  4d ( 6)                                   1.00000

179   55   Cs(1+)     [Kr] 4d(10) 5s(2) 5p(6)        1   :   4d-( 4)  4d ( 6)  5s ( 2)  5p-( 2)  5p ( 4)        1.00000

180   56   Ba(2+)     [Kr] 4d(10) 5s(2) 5p(6)        1   :   4d-( 4)  4d ( 6)  5s ( 2)  5p-( 2)  5p ( 4)        1.00000

181   57   La(2+)     [Xe] 5d(1)                     2   :   5d-( 1)                                            0.40000
                                                             5d ( 1)                                           0.60000
```

N.	Z	Atom	LS	n(CSF)	CSF	Weight(CSF)
182	57	La(3+)	[Kr] 4d(10) 5s(2) 5p(6)	1	: 4d-(4) 4d (6) 5s (2) 5p-(2) 5p (4)	1.00000
183	58	Ce(2+)	[Xe] 4f(2)	3	: 4f-(2)	0.16484
					4f-(1) 4f (1)	0.52747
					4f (2)	0.30769
184	58	Ce(3+)	[Xe] 4f(1)	2	: 4f-(1)	0.42857
					4f (1)	0.57143
185	58	Ce(4+)	[Kr] 4d(10) 5s(2) 5p(6)	1	: 4d-(4) 4d (6) 5s (2) 5p-(2) 5p (4)	1.00000
186	59	Pr(2+)	[Xe] 4f(3)	4	: 4f-(3)	0.05495
					4f-(2) 4f (1)	0.32967
					4f-(1) 4f (2)	0.46154
					4f (3)	0.15385
187	59	Pr(3+)	[Xe] 4f(2)	3	: 4f-(2)	0.16484
					4f-(1) 4f (1)	0.52747
					4f (2)	0.30769
188	59	Pr(4+)	[Xe] 4f(1)	2	: 4f-(1)	0.42857
					4f (1)	0.57143
189	60	Nd(2+)	[Xe] 4f(4)	5	: 4f-(4)	0.01499
					4f-(3) 4f (1)	0.15984
					4f-(2) 4f (2)	0.41958
					4f-(1) 4f (3)	0.33566
					4f (4)	0.06993
190	60	Nd(3+)	[Xe] 4f(3)	4	: 4f-(3)	0.05495
					4f-(2) 4f (1)	0.32967
					4f-(1) 4f (2)	0.46154
					4f (3)	0.15385
191	61	Pm(3+)	[Xe] 4f(4)	5	: 4f-(4)	0.01499

						4f-(3)	4f (1)	0.15984
						4f-(2)	4f (2)	0.41958
						4f-(1)	4f (3)	0.33566
						4f (4)		0.06993
192	62	Sm(2+)	[Xe] 4f(6)	7	:	4f-(6)		0.00033
						4f-(5)	4f (1)	0.01598
						4f-(4)	4f (2)	0.13986
						4f-(3)	4f (3)	0.37296
						4f-(2)	4f (4)	0.34965
						4f-(1)	4f (5)	0.11189
						4f (6)		0.00932

N.	Z	Atom	LS	n(CSF)		CSF				Weight(CSF)
193	62	Sm(3+)	[Xe] 4f(5)	6	:	4f-(5)				0.00300
						4f-(4)	4f (1)			0.05994
						4f-(3)	4f (2)			0.27972
						4f-(2)	4f (3)			0.41958
						4f-(1)	4f (4)			0.20979
						4f (5)				0.02797
194	63	Eu(2+)	[Xe] 4f(7)	7	:	4f-(6)	4f (1)			0.00233
						4f-(5)	4f (2)			0.04895
						4f-(4)	4f (3)			0.24476
						4f-(3)	4f (4)			0.40793
						4f-(2)	4f (5)			0.24476
						4f-(1)	4f (6)			0.04895
						4f (7)				0.00233
195	63	Eu(3+)	[Xe] 4f(6)	7	:	4f-(6)				0.00033
						4f-(5)	4f (1)			0.01598
						4f-(4)	4f (2)			0.13986
						4f-(3)	4f (3)			0.37296
						4f-(2)	4f (4)			0.34965
						4f-(1)	4f (5)			0.11189
						4f (6)				0.00932
196	64	Gd(1+)	[Xe] 4f(7) 5d(1) 6s(1)	14	:	4f-(6)	4f (1)	5d-(1)	6s (1)	0.00093
						4f-(6)	4f (1)	5d (1)	6s (1)	0.00140
						4f-(5)	4f (2)	5d-(1)	6s (1)	0.01958
						4f-(5)	4f (2)	5d (1)	6s (1)	0.02937
						4f-(4)	4f (3)	5d-(1)	6s (1)	0.09790
						4f-(4)	4f (3)	5d (1)	6s (1)	0.14685
						4f-(3)	4f (4)	5d-(1)	6s (1)	0.16317
						4f-(3)	4f (4)	5d (1)	6s (1)	0.24476
						4f-(2)	4f (5)	5d-(1)	6s (1)	0.09790
						4f-(2)	4f (5)	5d (1)	6s (1)	0.14685
						4f-(1)	4f (6)	5d-(1)	6s (1)	0.01958
						4f-(1)	4f (6)	5d (1)	6s (1)	0.02937

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4f ( 7)  5d-( 1)  6s ( 1)                                    0.00093
4f ( 7)  5d ( 1)  6s ( 1)                                    0.00140
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N.	Z	Atom	LS	n(CSF)		CSF			Weight(CSF)
197	64	Gd(2+)	[Xe] 4f(7) 5d(1)	14	:	4f-(6)	4f (1)	5d-(1)	0.00093
						4f-(6)	4f (1)	5d (1)	0.00140
						4f-(5)	4f (2)	5d-(1)	0.01958
						4f-(5)	4f (2)	5d (1)	0.02937
						4f-(4)	4f (3)	5d-(1)	0.09790
						4f-(4)	4f (3)	5d (1)	0.14685
						4f-(3)	4f (4)	5d-(1)	0.16317
						4f-(3)	4f (4)	5d (1)	0.24476
						4f-(2)	4f (5)	5d-(1)	0.09790
						4f-(2)	4f (5)	5d (1)	0.14685
						4f-(1)	4f (6)	5d-(1)	0.01958
						4f-(1)	4f (6)	5d (1)	0.02937
						4f (7)	5d-(1)		0.00093
						4f (7)	5d (1)		0.00140
198	64	Gd(3+)	[Xe] 4f(7)	7	:	4f-(6)	4f (1)		0.00233
						4f-(5)	4f (2)		0.04895
						4f-(4)	4f (3)		0.24476
						4f-(3)	4f (4)		0.40793
						4f-(2)	4f (5)		0.24476
						4f-(1)	4f (6)		0.04895
						4f (7)			0.00233
199	65	Tb(1+)	[Xe] 4f(9) 6s(1)	6	:	4f-(6)	4f (3)	6s (1)	0.02797
						4f-(5)	4f (4)	6s (1)	0.20979
						4f-(4)	4f (5)	6s (1)	0.41958
						4f-(3)	4f (6)	6s (1)	0.27972
						4f-(2)	4f (7)	6s (1)	0.05994
						4f-(1)	4f (8)	6s (1)	0.00300
200	65	Tb(3+)	[Xe] 4f(8)	7	:	4f-(6)	4f (2)		0.00932
						4f-(5)	4f (3)		0.11189
						4f-(4)	4f (4)		0.34965
						4f-(3)	4f (5)		0.37296
						4f-(2)	4f (6)		0.13986

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                                              4f-( 1)  4f ( 7)                    0.01598
                                              4f ( 8)                             0.00033


  201   65  Tb(4+)    [Xe] 4f(7)           7   :  4f-( 6)  4f ( 1)                0.00233
                                              4f-( 5)  4f ( 2)                    0.04895
                                              4f-( 4)  4f ( 3)                    0.24476
                                              4f-( 3)  4f ( 4)                    0.40793
                                              4f-( 2)  4f ( 5)                    0.24476
                                              4f-( 1)  4f ( 6)                    0.04895
                                              4f ( 7)                             0.00233
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N.	Z	Atom	LS	n(CSF)		CSF		Weight(CSF)
202	66	Dy(2+)	[Xe] 4f(10)	5	:	4f-(6)	4f (4)	0.06993
						4f-(5)	4f (5)	0.33566
						4f-(4)	4f (6)	0.41958
						4f-(3)	4f (7)	0.15984
						4f-(2)	4f (8)	0.01499
203	66	Dy(3+)	[Xe] 4f(9)	6	:	4f-(6)	4f (3)	0.02797
						4f-(5)	4f (4)	0.20979
						4f-(4)	4f (5)	0.41958
						4f-(3)	4f (6)	0.27972
						4f-(2)	4f (7)	0.05994
						4f-(1)	4f (8)	0.00300
204	67	Ho(3+)	[Xe] 4f(10)	5	:	4f-(6)	4f (4)	0.06993
						4f-(5)	4f (5)	0.33566
						4f-(4)	4f (6)	0.41958
						4f-(3)	4f (7)	0.15984
						4f-(2)	4f (8)	0.01499
205	68	Er(3+)	[Xe] 4f(11)	4	:	4f-(6)	4f (5)	0.15385
						4f-(5)	4f (6)	0.46154
						4f-(4)	4f (7)	0.32967
						4f-(3)	4f (8)	0.05495
206	69	Tm(2+)	[Xe] 4f(13)	2	:	4f-(6)	4f (7)	0.57143
						4f-(5)	4f (8)	0.42857
207	69	Tm(3+)	[Xe] 4f(12)	3	:	4f-(6)	4f (6)	0.30769
						4f-(5)	4f (7)	0.52747
						4f-(4)	4f (8)	0.16484
208	70	Yb(2+)	[Xe] 4f(14)	1	:	4f-(6)	4f (8)	1.00000
209	70	Yb(3+)	[Xe] 4f(13)	2	:	4f-(6)	4f (7)	0.57143
						4f-(5)	4f (8)	0.42857

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210   71  Lu(3+)    [Xe] 4f(14)                    1   :   4f-( 6)  4f ( 8)                              1.00000

211   72  Hf(2+)    [Xe] 4f(14) 5d(2)              3   :   4f-( 6)  4f ( 8)  5d-( 2)                     0.13333
                                                           4f-( 6)  4f ( 8)  5d-( 1)  5d ( 1)            0.53333
                                                           4f-( 6)  4f ( 8)  5d ( 2)                     0.33333

212   72  Hf(3+)    [Xe] 4f(14) 5d(1)              2   :   4f-( 6)  4f ( 8)  5d-( 1)                     0.40000
                                                           4f-( 6)  4f ( 8)  5d ( 1)                     0.60000

213   72  Hf(4+)    [Xe] 4f(14)                    1   :   4f-( 6)  4f ( 8)                              1.00000
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N.	Z	Atom	LS	n(CSF)		CSF				Weight(CSF)
214	73	Ta(2+)	[Xe] 4f(14) 5d(3)	4	:	4f-(6)	4f (8)	5d-(3)		0.03333
						4f-(6)	4f (8)	5d-(2)	5d (1)	0.30000
						4f-(6)	4f (8)	5d-(1)	5d (2)	0.50000
						4f-(6)	4f (8)	5d (3)		0.16667
215	73	Ta(3+)	[Xe] 4f(14) 5d(2)	3	:	4f-(6)	4f (8)	5d-(2)		0.13333
						4f-(6)	4f (8)	5d-(1)	5d (1)	0.53333
						4f-(6)	4f (8)	5d (2)		0.33333
216	73	Ta(4+)	[Xe] 4f(14) 5d(1)	2	:	4f-(6)	4f (8)	5d-(1)		0.40000
						4f-(6)	4f (8)	5d (1)		0.60000
217	73	Ta(5+)	[Xe] 4f(14)	1	:	4f-(6)	4f (8)			1.00000
218	74	W(1+)	[Xe] 4f(14) 5d(4) 6s(1)	5	:	4f-(6)	4f (8)	5d-(4)	6s (1)	0.00476
						4f-(6)	4f (8)	5d-(3)	5d (1) 6s (1)	0.11429
						4f-(6)	4f (8)	5d-(2)	5d (2) 6s (1)	0.42857
						4f-(6)	4f (8)	5d-(1)	5d (3) 6s (1)	0.38095
						4f-(6)	4f (8)	5d (4)	6s (1)	0.07143
219	74	W(2+)	[Xe] 4f(14) 5d(4)	5	:	4f-(6)	4f (8)	5d-(4)		0.00476
						4f-(6)	4f (8)	5d-(3)	5d (1)	0.11429
						4f-(6)	4f (8)	5d-(2)	5d (2)	0.42857
						4f-(6)	4f (8)	5d-(1)	5d (3)	0.38095
						4f-(6)	4f (8)	5d (4)		0.07143
220	74	W(3+)	[Xe] 4f(14) 5d(3)	4	:	4f-(6)	4f (8)	5d-(3)		0.03333
						4f-(6)	4f (8)	5d-(2)	5d (1)	0.30000
						4f-(6)	4f (8)	5d-(1)	5d (2)	0.50000
						4f-(6)	4f (8)	5d (3)		0.16667
221	74	W(4+)	[Xe] 4f(14) 5d(2)	3	:	4f-(6)	4f (8)	5d-(2)		0.13333
						4f-(6)	4f (8)	5d-(1)	5d (1)	0.53333
						4f-(6)	4f (8)	5d (2)		0.33333

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222    74   W(5+)      [Xe] 4f(14) 5d(1)             2   :   4f-( 6)   4f ( 8)   5d-( 1)                       0.40000
                                                             4f-( 6)   4f ( 8)   5d ( 1)                       0.60000


223    74   W(6+)      [Xe] 4f(14)                   1   :   4f-( 6)   4f ( 8)                                 1.00000


224    75   Re(1+)     [Xe] 4f(14) 5d(5) 6s(1)       5   :   4f-( 6)   4f ( 8)   5d-( 4)   5d ( 1)   6s ( 1)   0.02381
                                                             4f-( 6)   4f ( 8)   5d-( 3)   5d ( 2)   6s ( 1)   0.23810
                                                             4f-( 6)   4f ( 8)   5d-( 2)   5d ( 3)   6s ( 1)   0.47619
                                                             4f-( 6)   4f ( 8)   5d-( 1)   5d ( 4)   6s ( 1)   0.23810
                                                             4f-( 6)   4f ( 8)   5d ( 5)   6s ( 1)            0.02381
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N.	Z	Atom	LS	n(CSF)		CSF					Weight(CSF)
225	75	Re(2+)	[Xe] 4f(14) 5d(5)	5	:	4f-(6)	4f (8)	5d-(4)	5d (1)		0.02381
						4f-(6)	4f (8)	5d-(3)	5d (2)		0.23810
						4f-(6)	4f (8)	5d-(2)	5d (3)		0.47619
						4f-(6)	4f (8)	5d-(1)	5d (4)		0.23810
						4f-(6)	4f (8)	5d (5)			0.02381
226	75	Re(3+)	[Xe] 4f(14) 5d(4)	5	:	4f-(6)	4f (8)	5d-(4)			0.00476
						4f-(6)	4f (8)	5d-(3)	5d (1)		0.11429
						4f-(6)	4f (8)	5d-(2)	5d (2)		0.42857
						4f-(6)	4f (8)	5d-(1)	5d (3)		0.38095
						4f-(6)	4f (8)	5d (4)			0.07143
227	75	Re(4+)	[Xe] 4f(14) 5d(3)	4	:	4f-(6)	4f (8)	5d-(3)			0.03333
						4f-(6)	4f (8)	5d-(2)	5d (1)		0.30000
						4f-(6)	4f (8)	5d-(1)	5d (2)		0.50000
						4f-(6)	4f (8)	5d (3)			0.16667
228	75	Re(5+)	[Xe] 4f(14) 5d(2)	3	:	4f-(6)	4f (8)	5d-(2)			0.13333
						4f-(6)	4f (8)	5d-(1)	5d (1)		0.53333
						4f-(6)	4f (8)	5d (2)			0.33333
229	75	Re(6+)	[Xe] 4f(14) 5d(1)	2	:	4f-(6)	4f (8)	5d-(1)			0.40000
						4f-(6)	4f (8)	5d (1)			0.60000
230	75	Re(7+)	[Xe] 4f(14)	1	:	4f-(6)	4f (8)				1.00000
231	76	Os(1+)	[Xe] 4f(14) 5d(6) 6s(1)	5	:	4f-(6)	4f (8)	5d-(4)	5d (2)	6s (1)	0.07143
						4f-(6)	4f (8)	5d-(3)	5d (3)	6s (1)	0.38095
						4f-(6)	4f (8)	5d-(2)	5d (4)	6s (1)	0.42857
						4f-(6)	4f (8)	5d-(1)	5d (5)	6s (1)	0.11429
						4f-(6)	4f (8)	5d (6)	6s (1)		0.00476
232	76	Os(2+)	[Xe] 4f(14) 5d(6)	5	:	4f-(6)	4f (8)	5d-(4)	5d (2)		0.07143
						4f-(6)	4f (8)	5d-(3)	5d (3)		0.38095
						4f-(6)	4f (8)	5d-(2)	5d (4)		0.42857

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                                                     4f-( 6)  4f ( 8)  5d-( 1)  5d ( 5)                0.11429
                                                     4f-( 6)  4f ( 8)  5d ( 6)                         0.00476


   233   76  Os(3+)    [Xe] 4f(14) 5d(5)            5   :   4f-( 6)  4f ( 8)  5d-( 4)  5d ( 1)         0.02381
                                                     4f-( 6)  4f ( 8)  5d-( 3)  5d ( 2)                0.23810
                                                     4f-( 6)  4f ( 8)  5d-( 2)  5d ( 3)                0.47619
                                                     4f-( 6)  4f ( 8)  5d-( 1)  5d ( 4)                0.23810
                                                     4f-( 6)  4f ( 8)  5d ( 5)                         0.02381
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N.	Z	Atom	LS	n(CSF)		CSF					Weight(CSF)
234	76	Os(4+)	[Xe] 4f(14) 5d(4)	5	:	4f-(6)	4f (8)	5d-(4)			0.00476
						4f-(6)	4f (8)	5d-(3)	5d (1)		0.11429
						4f-(6)	4f (8)	5d-(2)	5d (2)		0.42857
						4f-(6)	4f (8)	5d-(1)	5d (3)		0.38095
						4f-(6)	4f (8)	5d (4)			0.07143
235	76	Os(5+)	[Xe] 4f(14) 5d(3)	4	:	4f-(6)	4f (8)	5d-(3)			0.03333
						4f-(6)	4f (8)	5d-(2)	5d (1)		0.30000
						4f-(6)	4f (8)	5d-(1)	5d (2)		0.50000
						4f-(6)	4f (8)	5d (3)			0.16667
236	76	Os(6+)	[Xe] 4f(14) 5d(2)	3	:	4f-(6)	4f (8)	5d-(2)			0.13333
						4f-(6)	4f (8)	5d-(1)	5d (1)		0.53333
						4f-(6)	4f (8)	5d (2)			0.33333
237	76	Os(7+)	[Xe] 4f(14) 5d(1)	2	:	4f-(6)	4f (8)	5d-(1)			0.40000
						4f-(6)	4f (8)	5d (1)			0.60000
238	76	Os(8+)	[Xe] 4f(14)	1	:	4f-(6)	4f (8)				1.00000
239	77	Ir(1+)	[Xe] 4f(14) 5d(7) 6s(1)	4	:	4f-(6)	4f (8)	5d-(4)	5d (3)	6s (1)	0.16667
						4f-(6)	4f (8)	5d-(3)	5d (4)	6s (1)	0.50000
						4f-(6)	4f (8)	5d-(2)	5d (5)	6s (1)	0.30000
						4f-(6)	4f (8)	5d-(1)	5d (6)	6s (1)	0.03333
240	77	Ir(2+)	[Xe] 4f(14) 5d(7)	4	:	4f-(6)	4f (8)	5d-(4)	5d (3)		0.16667
						4f-(6)	4f (8)	5d-(3)	5d (4)		0.50000
						4f-(6)	4f (8)	5d-(2)	5d (5)		0.30000
						4f-(6)	4f (8)	5d-(1)	5d (6)		0.03333
241	77	Ir(3+)	[Xe] 4f(14) 5d(6)	5	:	4f-(6)	4f (8)	5d-(4)	5d (2)		0.07143
						4f-(6)	4f (8)	5d-(3)	5d (3)		0.38095
						4f-(6)	4f (8)	5d-(2)	5d (4)		0.42857
						4f-(6)	4f (8)	5d-(1)	5d (5)		0.11429
						4f-(6)	4f (8)	5d (6)			0.00476

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242   77  Ir(4+)    [Xe] 4f(14) 5d(5)              5   :   4f-( 6)  4f ( 8)  5d-( 4)  5d ( 1)                   0.02381
                                                           4f-( 6)  4f ( 8)  5d-( 3)  5d ( 2)                   0.23810
                                                           4f-( 6)  4f ( 8)  5d-( 2)  5d ( 3)                   0.47619
                                                           4f-( 6)  4f ( 8)  5d-( 1)  5d ( 4)                   0.23810
                                                           4f-( 6)  4f ( 8)  5d ( 5)                            0.02381


243   77  Ir(5+)    [Xe] 4f(14) 5d(4)              5   :   4f-( 6)  4f ( 8)  5d-( 4)                            0.00476
                                                           4f-( 6)  4f ( 8)  5d-( 3)  5d ( 1)                   0.11429
                                                           4f-( 6)  4f ( 8)  5d-( 2)  5d ( 2)                   0.42857
                                                           4f-( 6)  4f ( 8)  5d-( 1)  5d ( 3)                   0.38095
                                                           4f-( 6)  4f ( 8)  5d ( 4)                            0.07143
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N.	Z	Atom	LS	n(CSF)		CSF				Weight(CSF)
244	77	Ir(6+)	[Xe] 4f(14) 5d(3)	4	:	4f-(6)	4f (8)	5d-(3)		0.03333
						4f-(6)	4f (8)	5d-(2)	5d (1)	0.30000
						4f-(6)	4f (8)	5d-(1)	5d (2)	0.50000
						4f-(6)	4f (8)	5d (3)		0.16667
245	78	Pt(2+)	[Xe] 4f(14) 5d(8)	3	:	4f-(6)	4f (8)	5d-(4)	5d (4)	0.33333
						4f-(6)	4f (8)	5d-(3)	5d (5)	0.53333
						4f-(6)	4f (8)	5d-(2)	5d (6)	0.13333
246	78	Pt(4+)	[Xe] 4f(14) 5d(6)	5	:	4f-(6)	4f (8)	5d-(4)	5d (2)	0.07143
						4f-(6)	4f (8)	5d-(3)	5d (3)	0.38095
						4f-(6)	4f (8)	5d-(2)	5d (4)	0.42857
						4f-(6)	4f (8)	5d-(1)	5d (5)	0.11429
						4f-(6)	4f (8)	5d (6)		0.00476
247	78	Pt(5+)	[Xe] 4f(14) 5d(5)	5	:	4f-(6)	4f (8)	5d-(4)	5d (1)	0.02381
						4f-(6)	4f (8)	5d-(3)	5d (2)	0.23810
						4f-(6)	4f (8)	5d-(2)	5d (3)	0.47619
						4f-(6)	4f (8)	5d-(1)	5d (4)	0.23810
						4f-(6)	4f (8)	5d (5)		0.02381
248	78	Pt(6+)	[Xe] 4f(14) 5d(4)	5	:	4f-(6)	4f (8)	5d-(4)		0.00476
						4f-(6)	4f (8)	5d-(3)	5d (1)	0.11429
						4f-(6)	4f (8)	5d-(2)	5d (2)	0.42857
						4f-(6)	4f (8)	5d-(1)	5d (3)	0.38095
						4f-(6)	4f (8)	5d (4)		0.07143
249	79	Au(1+)	[Xe] 4f(14) 5d(10)	1	:	4f-(6)	4f (8)	5d-(4)	5d (6)	1.00000
250	79	Au(2+)	[Xe] 4f(14) 5d(9)	2	:	4f-(6)	4f (8)	5d-(4)	5d (5)	0.60000
						4f-(6)	4f (8)	5d-(3)	5d (6)	0.40000
251	79	Au(3+)	[Xe] 4f(14) 5d(8)	3	:	4f-(6)	4f (8)	5d-(4)	5d (4)	0.33333
						4f-(6)	4f (8)	5d-(3)	5d (5)	0.53333
						4f-(6)	4f (8)	5d-(2)	5d (6)	0.13333

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252   79  Au(5+)    [Xe] 4f(14) 5d(6)          5   :   4f-( 6)  4f ( 8)  5d-( 4)  5d ( 2)                    0.07143
                                                       4f-( 6)  4f ( 8)  5d-( 3)  5d ( 3)                    0.38095
                                                       4f-( 6)  4f ( 8)  5d-( 2)  5d ( 4)                    0.42857
                                                       4f-( 6)  4f ( 8)  5d-( 1)  5d ( 5)                    0.11429
                                                       4f-( 6)  4f ( 8)  5d ( 6)                             0.00476


253   80  Hg(1+)    [Xe] 4f(14) 5d(10) 6s(1)    1   :   4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 1)          1.00000


254   80  Hg(2+)    [Xe] 4f(14) 5d(10)          1   :   4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)                   1.00000


255   81  Tl(1+)    [Xe] 4f(14) 5d(10) 6s(2)    1   :   4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)          1.00000
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  N.    Z  Atom    LS                              n(CSF)    CSF                                                                    Weight(CSF)
  ---------------------------------------------------------------------------------------------------------------------------------------------
  256  81  Tl(3+)  [Xe] 4f(14) 5d(10)                 1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)                                       1.00000

  257  82  Pb(2+)  [Xe] 4f(14) 5d(10) 6s(2)           1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)                              1.00000

  258  82  Pb(4+)  [Xe] 4f(14) 5d(10)                 1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)                                       1.00000

  259  83  Bi(3+)  [Xe] 4f(14) 5d(10) 6s(2)           1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)                              1.00000

  260  83  Bi(5+)  [Xe] 4f(14) 5d(10)                 1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)                                       1.00000

  261  84  Po(2+)  [Xe] 4f(14) 5d(10) 6s(2) 6p(2)     3   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 2)                     0.06667
                                                             4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 1)  6p ( 1)           0.53333
                                                             4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p ( 2)                    0.40000

  262  84  Po(4+)  [Xe] 4f(14) 5d(10) 6s(2)           1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)                              1.00000

  263  84  Po(6+)  [Xe] 4f(14) 5d(10)                 1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)                                       1.00000

  264  85  At(1+)  [Xe] 4f(14) 5d(10) 6s(2) 6p(4)     3   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 2)  6p ( 2)           0.40000
                                                             4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 1)  6p ( 3)           0.53333
                                                             4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p ( 4)                    0.06667

  265  85  At(3+)  [Xe] 4f(14) 5d(10) 6s(2) 6p(2)     3   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 2)                     0.06667
                                                             4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 1)  6p ( 1)           0.53333
                                                             4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p ( 2)                    0.40000

  266  85  At(5+)  [Xe] 4f(14) 5d(10) 6s(2)           1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)                              1.00000

  267  85  At(7+)  [Xe] 4f(14) 5d(10)                 1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)                                       1.00000

  268  85  At(1-)  [Xe] 4f(14) 5d(10) 6s(2) 6p(6)     1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 2)  6p ( 4)           1.00000

  269  87  Fr(1+)  [Xe] 4f(14) 5d(10) 6s(2) 6p(6)     1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 2)  6p ( 4)           1.00000

  270  88  Ra(2+)  [Xe] 4f(14) 5d(10) 6s(2) 6p(6)     1   :  4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 2)  6p ( 4)           1.00000
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271	89	Ac(3+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	1	:	4f-(6)	4f (8)	5d-(4)	5d (6)	6s (2)	6p-(2)	6p (4)	1.00000
272	90	Th(2+)	[Rn] 6d(1) 5f(1)	4	:	6d-(1)	5f-(1)						0.17143
						6d-(1)	5f (1)						0.22857
						6d (1)	5f-(1)						0.25714
						6d (1)	5f (1)						0.34286
273	90	Th(3+)	[Rn] 5f(1)	2	:	5f-(1)							0.42857
						5f (1)							0.57143
274	90	Th(4+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	1	:	4f-(6)	4f (8)	5d-(4)	5d (6)	6s (2)	6p-(2)	6p (4)	1.00000

N.	Z	Atom	LS	n(CSF)		CSF											Weight(CSF)
275	91	Pa(3+)	[Rn] 5f(2)	3	:	5f-(2)											0.16484
						5f-(1)	5f (1)										0.52747
						5f (2)											0.30769
276	91	Pa(4+)	[Rn] 5f(1)	2	:	5f-(1)											0.42857
						5f (1)											0.57143
277	91	Pa(5+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	1	:	4f-(6)	4f (8)	5d-(4)	5d (6)	6s (2)	6p-(2)	6p (4)					1.00000
278	92	U(3+)	[Rn] 5f(3)	4	:	5f-(3)											0.05495
						5f-(2)	5f (1)										0.32967
						5f-(1)	5f (2)										0.46154
						5f (3)											0.15385
279	92	U(4+)	[Rn] 5f(2)	3	:	5f-(2)											0.16484
						5f-(1)	5f (1)										0.52747
						5f (2)											0.30769
280	92	U(5+)	[Rn] 5f(1)	2	:	5f-(1)											0.42857
						5f (1)											0.57143
281	92	U(6+)	[Xe] 4f(14) 5d(10) 6s(2) 6p(6)	1	:	4f-(6)	4f (8)	5d-(4)	5d (6)	6s (2)	6p-(2)	6p (4)					1.00000
282	93	Np(3+)	[Rn] 5f(4)	5	:	5f-(4)											0.01499
						5f-(3)	5f (1)										0.15984
						5f-(2)	5f (2)										0.41958
						5f-(1)	5f (3)										0.33566
						5f (4)											0.06993
283	93	Np(4+)	[Rn] 5f(3)	4	:	5f-(3)											0.05495
						5f-(2)	5f (1)										0.32967
						5f-(1)	5f (2)										0.46154
						5f (3)											0.15385
284	93	Np(5+)	[Rn] 5f(2)	3	:	5f-(2)											0.16484

```
                                                    5f-( 1)  5f ( 1)                                          0.52747
                                                    5f ( 2)                                                   0.30769


   285    93  Np(6+)    [Rn] 5f(1)                 2   :   5f-( 1)                                             0.42857
                                                    5f ( 1)                                                   0.57143


   286    93  Np(7+)    [Xe] 4f(14) 5d(10) 6s(2) 6p(6)   1   :   4f-( 6)  4f ( 8)  5d-( 4)  5d ( 6)  6s ( 2)  6p-( 2)  6p ( 4)    1.00000
```

N.	Z	Atom	LS	n(CSF)		CSF		Weight(CSF)
287	94	Pu(3+)	[Rn] 5f(5)	6	:	5f-(5)		0.00300
						5f-(4)	5f (1)	0.05994
						5f-(3)	5f (2)	0.27972
						5f-(2)	5f (3)	0.41958
						5f-(1)	5f (4)	0.20979
						5f (5)		0.02797
288	94	Pu(4+)	[Rn] 5f(4)	5	:	5f-(4)		0.01499
						5f-(3)	5f (1)	0.15984
						5f-(2)	5f (2)	0.41958
						5f-(1)	5f (3)	0.33566
						5f (4)		0.06993
289	94	Pu(5+)	[Rn] 5f(3)	4	:	5f-(3)		0.05495
						5f-(2)	5f (1)	0.32967
						5f-(1)	5f (2)	0.46154
						5f (3)		0.15385
290	94	Pu(6+)	[Rn] 5f(2)	3	:	5f-(2)		0.16484
						5f-(1)	5f (1)	0.52747
						5f (2)		0.30769
291	94	Pu(7+)	[Rn] 5f(1)	2	:	5f-(1)		0.42857
						5f (1)		0.57143
292	95	Am(2+)	[Rn] 5f(7)	7	:	5f-(6)	5f (1)	0.00233
						5f-(5)	5f (2)	0.04895
						5f-(4)	5f (3)	0.24476
						5f-(3)	5f (4)	0.40793
						5f-(2)	5f (5)	0.24476
						5f-(1)	5f (6)	0.04895
						5f (7)		0.00233
293	95	Am(3+)	[Rn] 5f(6)	7	:	5f-(6)		0.00033
						5f-(5)	5f (1)	0.01598

```
                                          5f-( 4)  5f ( 2)                    0.13986
                                          5f-( 3)  5f ( 3)                    0.37296
                                          5f-( 2)  5f ( 4)                    0.34965
                                          5f-( 1)  5f ( 5)                    0.11189
                                          5f ( 6)                             0.00932


  294   95  Am(4+)    [Rn] 5f(5)          6  :   5f-( 5)                      0.00300
                                          5f-( 4)  5f ( 1)                    0.05994
                                          5f-( 3)  5f ( 2)                    0.27972
                                          5f-( 2)  5f ( 3)                    0.41958
                                          5f-( 1)  5f ( 4)                    0.20979
                                          5f ( 5)                             0.02797
```

N.	Z	Atom	LS	n(CSF)		CSF		Weight(CSF)
295	95	Am(5+)	[Rn] 5f(4)	5	:	5f-(4)		0.01499
						5f-(3)	5f (1)	0.15984
						5f-(2)	5f (2)	0.41958
						5f-(1)	5f (3)	0.33566
						5f (4)		0.06993
296	95	Am(6+)	[Rn] 5f(3)	4	:	5f-(3)		0.05495
						5f-(2)	5f (1)	0.32967
						5f-(1)	5f (2)	0.46154
						5f (3)		0.15385
297	96	Cm(3+)	[Rn] 5f(7)	7	:	5f-(6)	5f (1)	0.00233
						5f-(5)	5f (2)	0.04895
						5f-(4)	5f (3)	0.24476
						5f-(3)	5f (4)	0.40793
						5f-(2)	5f (5)	0.24476
						5f-(1)	5f (6)	0.04895
						5f (7)		0.00233
298	96	Cm(4+)	[Rn] 5f(6)	7	:	5f-(6)		0.00033
						5f-(5)	5f (1)	0.01598
						5f-(4)	5f (2)	0.13986
						5f-(3)	5f (3)	0.37296
						5f-(2)	5f (4)	0.34965
						5f-(1)	5f (5)	0.11189
						5f (6)		0.00932
299	97	Bk(3+)	[Rn] 5f(8)	7	:	5f-(6)	5f (2)	0.00932
						5f-(5)	5f (3)	0.11189
						5f-(4)	5f (4)	0.34965
						5f-(3)	5f (5)	0.37296
						5f-(2)	5f (6)	0.13986
						5f-(1)	5f (7)	0.01598
						5f (8)		0.00033

```
300   97  Bk(4+)    [Rn] 5f(7)                      7   :   5f-( 6)  5f ( 1)                              0.00233
                                                            5f-( 5)  5f ( 2)                              0.04895
                                                            5f-( 4)  5f ( 3)                              0.24476
                                                            5f-( 3)  5f ( 4)                              0.40793
                                                            5f-( 2)  5f ( 5)                              0.24476
                                                            5f-( 1)  5f ( 6)                              0.04895
                                                            5f ( 7)                                       0.00233
```

N.	Z	Atom	LS	n(CSF)	CSF		Weight(CSF)
301	98	Cf(2+)	[Rn] 5f(10)	5 :	5f-(6)	5f (4)	0.06993
					5f-(5)	5f (5)	0.33566
					5f-(4)	5f (6)	0.41958
					5f-(3)	5f (7)	0.15984
					5f-(2)	5f (8)	0.01499
302	98	Cf(3+)	[Rn] 5f(9)	6 :	5f-(6)	5f (3)	0.02797
					5f-(5)	5f (4)	0.20979
					5f-(4)	5f (5)	0.41958
					5f-(3)	5f (6)	0.27972
					5f-(2)	5f (7)	0.05994
					5f-(1)	5f (8)	0.00300
303	98	Cf(4+)	[Rn] 5f(8)	7 :	5f-(6)	5f (2)	0.00932
					5f-(5)	5f (3)	0.11189
					5f-(4)	5f (4)	0.34965
					5f-(3)	5f (5)	0.37296
					5f-(2)	5f (6)	0.13986
					5f-(1)	5f (7)	0.01598
					5f (8)		0.00033
304	99	Es(2+)	[Rn] 5f(11)	4 :	5f-(6)	5f (5)	0.15385
					5f-(5)	5f (6)	0.46154
					5f-(4)	5f (7)	0.32967
					5f-(3)	5f (8)	0.05495
305	99	Es(3+)	[Rn] 5f(10)	5 :	5f-(6)	5f (4)	0.06993
					5f-(5)	5f (5)	0.33566
					5f-(4)	5f (6)	0.41958
					5f-(3)	5f (7)	0.15984
					5f-(2)	5f (8)	0.01499
306	100	Fm(2+)	[Rn] 5f(12)	3 :	5f-(6)	5f (6)	0.30769
					5f-(5)	5f (7)	0.52747
					5f-(4)	5f (8)	0.16484

```
307  100  Fm(3+)    [Rn] 5f(11)              4   :   5f-( 6)  5f ( 5)                          0.15385
                                                     5f-( 5)  5f ( 6)                          0.46154
                                                     5f-( 4)  5f ( 7)                          0.32967
                                                     5f-( 3)  5f ( 8)                          0.05495


308  101  Md(2+)    [Rn] 5f(13)              2   :   5f-( 6)  5f ( 7)                          0.57143
                                                     5f-( 5)  5f ( 8)                          0.42857


309  101  Md(3+)    [Rn] 5f(12)              3   :   5f-( 6)  5f ( 6)                          0.30769
                                                     5f-( 5)  5f ( 7)                          0.52747
                                                     5f-( 4)  5f ( 8)                          0.16484
```

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  N.    Z  Atom     LS                      n(CSF)    CSF                                                      Weight(CSF)
------------------------------------------------------------------------------------------------------------------------

 310  102  No(2+)   [Rn] 5f(14)                1   :  5f-( 6)  5f ( 8)                                            1.00000


 311  102  No(3+)   [Rn] 5f(13)                2   :  5f-( 6)  5f ( 7)                                            0.57143
                                                      5f-( 5)  5f ( 8)                                            0.42857


 312  103  Lr(3+)   [Rn] 5f(14)                1   :  5f-( 6)  5f ( 8)                                            1.00000


 313  104  Rf(4+)   [Rn] 5f(14)                1   :  5f-( 6)  5f ( 8)                                            1.00000


 314  105  Db(5+)   [Rn] 5f(14)                1   :  5f-( 6)  5f ( 8)                                            1.00000


 315  106  Sg(6+)   [Rn] 5f(14)                1   :  5f-( 6)  5f ( 8)                                            1.00000


 316  107  Bh(7+)   [Rn] 5f(14)                1   :  5f-( 6)  5f ( 8)                                            1.00000


 317  108  Hs(8+)   [Rn] 5f(14)                1   :  5f-( 6)  5f ( 8)                                            1.00000


 318  112  Cn(2+)   [Rn] 5f(14) 6d(10)        1   :  5f-( 6)  5f ( 8)  6d-( 4)  6d ( 6)                          1.00000
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Table S3. Mean atomic scattering factors in electrons for all species calculated in this work.
Method: DHF - relativistic Dirac-Hartree-Fock (DBSR_HF)
STL - sin(theta)/lambda in reciprocal angstroms
DATE = 2022-08-11   TIME = 19:01:30

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Atom	Li(1+)	Be(2+)	B(1+)	B(2+)	B(3+)	C(1+)	C(2+)	C(3+)	C(4+)
Z	3	4	5	5	5	6	6	6	6
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL									
0.00	2.00000	2.00000	4.00000	3.00000	2.00000	5.00000	4.00000	3.00000	2.00000
0.01	1.99934	1.99966	3.99416	2.99749	1.99979	4.99407	3.99660	2.99845	1.99986
0.02	1.99738	1.99863	3.97675	2.98999	1.99916	4.97636	3.98643	2.99382	1.99944
0.03	1.99411	1.99693	3.94807	2.97760	1.99812	4.94710	3.96960	2.98614	1.99873
0.04	1.98954	1.99455	3.90861	2.96047	1.99666	4.90665	3.94626	2.97546	1.99775
0.05	1.98370	1.99149	3.85905	2.93883	1.99479	4.85554	3.91664	2.96188	1.99648
0.06	1.97659	1.98776	3.80018	2.91294	1.99250	4.79439	3.88103	2.94550	1.99494
0.07	1.96825	1.98337	3.73297	2.88311	1.98980	4.72395	3.83975	2.92643	1.99311
0.08	1.95869	1.97832	3.65845	2.84969	1.98669	4.64504	3.79318	2.90482	1.99101
0.09	1.94794	1.97263	3.57772	2.81307	1.98318	4.55856	3.74176	2.88083	1.98863
0.10	1.93604	1.96629	3.49193	2.77366	1.97927	4.46547	3.68591	2.85462	1.98598
0.11	1.92303	1.95932	3.40222	2.73187	1.97495	4.36673	3.62613	2.82638	1.98306
0.12	1.90893	1.95174	3.30971	2.68812	1.97025	4.26335	3.56290	2.79630	1.97986
0.13	1.89379	1.94355	3.21549	2.64284	1.96515	4.15631	3.49672	2.76457	1.97640
0.14	1.87766	1.93476	3.12058	2.59644	1.95967	4.04656	3.42810	2.73139	1.97267
0.15	1.86057	1.92539	3.02589	2.54931	1.95381	3.93503	3.35754	2.69698	1.96867
0.16	1.84257	1.91545	2.93228	2.50182	1.94758	3.82258	3.28553	2.66152	1.96441
0.17	1.82372	1.90496	2.84047	2.45431	1.94098	3.71004	3.21254	2.62523	1.95990
0.18	1.80406	1.89393	2.75110	2.40712	1.93401	3.59814	3.13902	2.58829	1.95513
0.19	1.78363	1.88238	2.66469	2.36051	1.92669	3.48756	3.06540	2.55089	1.95010
0.20	1.76250	1.87032	2.58166	2.31473	1.91902	3.37889	2.99207	2.51321	1.94482
0.22	1.71832	1.84476	2.42694	2.22651	1.90267	3.16927	2.84772	2.43770	1.93354
0.24	1.67191	1.81739	2.28846	2.14374	1.88500	2.97253	2.70848	2.36297	1.92129
0.25	1.64800	1.80307	2.22545	2.10467	1.87569	2.87970	2.64141	2.32624	1.91481
0.26	1.62369	1.78835	2.16655	2.06721	1.86607	2.79080	2.57631	2.29007	1.90811
0.28	1.57404	1.75779	2.06062	1.99724	1.84597	2.62519	2.45259	2.21983	1.89403
0.30	1.52335	1.72587	1.96948	1.93380	1.82475	2.47602	2.33822	2.15286	1.87909
0.32	1.47197	1.69274	1.89157	1.87658	1.80247	2.34298	2.23363	2.08960	1.86332
0.34	1.42023	1.65854	1.82516	1.82506	1.77922	2.22526	2.13886	2.03029	1.84675
0.35	1.39432	1.64110	1.79572	1.80126	1.76726	2.17182	2.09510	2.00215	1.83818
0.36	1.36843	1.62345	1.76850	1.77864	1.75507	2.12179	2.05368	1.97503	1.82942
0.38	1.31685	1.58759	1.71992	1.73663	1.73008	2.03126	1.97759	1.92377	1.81138
0.40	1.26574	1.55111	1.67788	1.69835	1.70434	1.95231	1.90996	1.87639	1.79266
0.42	1.21532	1.51416	1.64103	1.66315	1.67790	1.88356	1.85004	1.83266	1.77329
0.44	1.16576	1.47686	1.60820	1.63044	1.65086	1.82366	1.79703	1.79230	1.75332
0.45	1.14136	1.45812	1.59297	1.61485	1.63713	1.79664	1.77287	1.77330	1.74313
0.46	1.11723	1.43934	1.57840	1.59968	1.62327	1.77137	1.75013	1.75502	1.73280
0.48	1.06986	1.40171	1.55084	1.57041	1.59521	1.72551	1.70852	1.72048	1.71175
0.50	1.02377	1.36409	1.52484	1.54224	1.56675	1.68507	1.67147	1.68835	1.69023
0.55	0.91461	1.27073	1.46362	1.47472	1.49427	1.60184	1.59430	1.61651	1.63458
0.60	0.81471	1.17944	1.40402	1.40891	1.42067	1.53557	1.53216	1.55332	1.57680
0.65	0.72428	1.09129	1.34368	1.34322	1.34685	1.47863	1.47844	1.49529	1.51750
0.70	0.64313	1.00709	1.28194	1.27722	1.27357	1.42624	1.42872	1.43996	1.45721
0.80	0.50655	0.85254	1.15552	1.14530	1.13123	1.32526	1.33189	1.33204	1.33575
0.90	0.39963	0.71782	1.02967	1.01699	0.99761	1.22341	1.23272	1.22447	1.21597
1.00	0.31659	0.60268	0.90951	0.89624	0.87509	1.12040	1.13114	1.11758	1.10060
1.10	0.25224	0.50559	0.79839	0.78559	0.76473	1.01860	1.02980	1.01343	0.99157
1.20	0.20228	0.42442	0.69800	0.68618	0.66668	0.92054	0.93154	0.91412	0.89010
1.30	0.16335	0.35692	0.60877	0.59813	0.58044	0.82810	0.83852	0.82118	0.79682
1.40	0.13286	0.30091	0.53036	0.52092	0.50516	0.74245	0.75208	0.73549	0.71193
1.50	0.10882	0.25448	0.46198	0.45368	0.43978	0.66412	0.67288	0.65741	0.63526
1.60	0.08974	0.21596	0.40266	0.39540	0.38321	0.59319	0.60108	0.58688	0.56646
1.70	0.07451	0.18394	0.35135	0.34502	0.33437	0.52944	0.53649	0.52360	0.50499
1.80	0.06226	0.15726	0.30707	0.30154	0.29224	0.47244	0.47873	0.46710	0.45027
1.90	0.05234	0.13497	0.26887	0.26404	0.25592	0.42168	0.42727	0.41683	0.40170
2.00	0.04426	0.11629	0.23591	0.23169	0.22459	0.37660	0.38156	0.37221	0.35864
2.50	0.02070	0.05835	0.12702	0.12480	0.12105	0.21758	0.22034	0.21498	0.20719
3.00	0.01079	0.03181	0.07257	0.07133	0.06922	0.13053	0.13212	0.12897	0.12437
3.50	0.00611	0.01858	0.04380	0.04306	0.04180	0.08156	0.08253	0.08059	0.07776
4.00	0.00370	0.01149	0.02773	0.02726	0.02648	0.05297	0.05359	0.05234	0.05053
5.00	0.00158	0.00503	0.01250	0.01229	0.01194	0.02470	0.02498	0.02441	0.02358
6.00	0.00078	0.00251	0.00637	0.00626	0.00609	0.01284	0.01299	0.01269	0.01227

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------------------------------------------------ Page   2 ------------------------------------------------
Atom     C(val)     N(1+)      N(2+)      N(3+)      N(4+)      N(5+)      O(1+)      O(2+)      O(1-)      F(1-)
   Z         6          7          7          7          7          7          8          8          8          9
Method      DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
  STL
  0.00    6.00000    6.00000    5.00000    4.00000    3.00000    2.00000    7.00000    6.00000    9.00000   10.00000
  0.01    5.98894    5.99424    4.99634    3.99776    2.99895    1.99990    6.99449    5.99626    8.98619    9.98824
  0.02    5.95599    5.97700    4.98540    3.99107    2.99580    1.99959    6.97799    5.98508    8.94510    9.95316
  0.03    5.90190    5.94847    4.96726    3.97996    2.99056    1.99909    6.95065    5.96652    8.87766    9.89536
  0.04    5.82784    5.90893    4.94206    3.96450    2.98327    1.99838    6.91268    5.94070    8.78537    9.81580
  0.05    5.73539    5.85876    4.90998    3.94479    2.97396    1.99747    6.86438    5.90778    8.67021    9.71576

  0.06    5.62642    5.79846    4.87128    3.92095    2.96268    1.99635    6.80612    5.86795    8.53444    9.59677
  0.07    5.50304    5.72859    4.82622    3.89313    2.94948    1.99504    6.73837    5.82146    8.38059    9.46055
  0.08    5.36751    5.64981    4.77515    3.86149    2.93444    1.99353    6.66162    5.76859    8.21123    9.30896
  0.09    5.22215    5.56282    4.71843    3.82623    2.91763    1.99181    6.57646    5.70964    8.02897    9.14390
  0.10    5.06925    5.46840    4.65645    3.78756    2.89912    1.98990    6.48348    5.64495    7.83631    8.96727

  0.11    4.91102    5.36735    4.58964    3.74569    2.87901    1.98779    6.38335    5.57490    7.63559    8.78096
  0.12    4.74951    5.26048    4.51844    3.70086    2.85740    1.98548    6.27674    5.49987    7.42899    8.58675
  0.13    4.58663    5.14865    4.44332    3.65333    2.83438    1.98297    6.16435    5.42026    7.21848    8.38634
  0.14    4.42405    5.03268    4.36474    3.60335    2.81007    1.98027    6.04690    5.33649    7.00579    8.18130
  0.15    4.26324    4.91340    4.28318    3.55117    2.78456    1.97738    5.92508    5.24899    6.79248    7.97305

  0.16    4.10545    4.79162    4.19911    3.49707    2.75796    1.97430    5.79962    5.15819    6.57988    7.76290
  0.17    3.95172    4.66810    4.11300    3.44132    2.73040    1.97102    5.67120    5.06453    6.36914    7.55203
  0.18    3.80286    4.54358    4.02531    3.38418    2.70198    1.96755    5.54049    4.96843    6.16123    7.34145
  0.19    3.65951    4.41874    3.93648    3.32590    2.67282    1.96390    5.40814    4.87033    5.95696    7.13208
  0.20    3.52216    4.29422    3.84695    3.26676    2.64302    1.96006    5.27476    4.77062    5.75700    6.92472

  0.22    3.26655    4.04843    3.66736    3.14685    2.58196    1.95183    5.00721    4.56804    5.37213    6.51863
  0.24    3.03716    3.81023    3.48948    3.02632    2.51965    1.94287    4.74204    4.36371    5.00973    6.12751
  0.25    2.93222    3.69499    3.40200    2.96636    2.48827    1.93813    4.61148    4.26176    4.83754    5.93855
  0.26    2.83362    3.58274    3.31587    2.90686    2.45688    1.93321    4.48279    4.16038    4.67155    5.75437
  0.28    2.65460    3.36822    3.14857    2.78994    2.39435    1.92285    4.23232    3.96043    4.35832    5.40118
  0.30    2.49816    3.16818    2.98922    2.67679    2.33270    1.91183    3.99286    3.76590    4.07000    5.06905

  0.32    2.36208    2.98343    2.83898    2.56841    2.27245    1.90015    3.76602    3.57843    3.80599    4.75846
  0.34    2.24405    2.81424    2.69864    2.46556    2.21406    1.88784    3.55288    3.39932    3.56532    4.46939
  0.35    2.19109    2.73544    2.63232    2.41638    2.18566    1.88145    3.45165    3.31321    3.45336    4.33281
  0.36    2.14179    2.66042    2.56860    2.36877    2.15785    1.87491    3.35403    3.22952    3.34676    4.20144
  0.38    2.05317    2.52146    2.44900    2.27837    2.10410    1.86139    3.16970    3.06967    3.14892    3.95394
  0.40    1.97622    2.39657    2.33968    2.19450    2.05296    1.84731    2.99977    2.92014    2.97032    3.72604

  0.42    1.90918    2.28481    2.24031    2.11716    2.00455    1.83267    2.84387    2.78104    2.80947    3.51674
  0.44    1.85048    2.18517    2.15042    2.04621    1.95887    1.81752    2.70145    2.65230    2.66487    3.32496
  0.45    1.82382    2.13954    2.10884    2.01305    1.93706    1.80975    2.63508    2.59175    2.59821    3.23530
  0.46    1.79876    2.09654    2.06940    1.98140    1.91591    1.80186    2.57182    2.53369    2.53507    3.14960
  0.48    1.75283    2.01784    1.99660    1.92242    1.87560    1.78573    2.45418    2.42485    2.41869    2.98952
  0.50    1.71169    1.94802    1.93132    1.86889    1.83781    1.76914    2.34771    2.32530    2.31442    2.84360

  0.55    1.62443    1.80584    1.79640    1.75613    1.75343    1.72586    2.12470    2.11355    2.09889    2.53370
  0.60    1.55194    1.69910    1.69352    1.66799    1.68128    1.68030    1.95287    1.94739    1.93486    2.28973
  0.65    1.48782    1.61677    1.61352    1.59800    1.61853    1.63283    1.82036    1.81758    1.80893    2.09793
  0.70    1.42822    1.55064    1.54910    1.54058    1.56256    1.58384    1.71720    1.71571    1.71068    1.94675
  0.80    1.31483    1.44516    1.44652    1.44697    1.46273    1.48272    1.56878    1.56859    1.56751    1.73053
  0.90    1.20445    1.35472    1.35865    1.36447    1.37001    1.37962    1.46370    1.46481    1.46359    1.58667
  1.00    1.09658    1.26786    1.27385    1.28298    1.27902    1.27685    1.37799    1.38060    1.37705    1.48214

  1.10    0.99271    1.18115    1.18855    1.19960    1.18838    1.17632    1.29979    1.30385    1.29737    1.39787
  1.20    0.89446    1.09457    1.10278    1.11474    1.09864    1.07950    1.22397    1.22921    1.22009    1.32341
  1.30    0.80298    1.00932    1.01784    1.03000    1.01103    0.98744    1.14886    1.15493    1.14380    1.25342
  1.40    0.71894    0.92674    0.93519    0.94709    0.92677    0.90086    1.07441    1.08097    1.06855    1.18545
  1.50    0.64252    0.84796    0.85610    0.86743    0.84683    0.82017    1.00123    1.00801    0.99490    1.11863

  1.60    0.57359    0.77375    0.78145    0.79204    0.77188    0.74552    0.93009    0.93685    0.92356    1.05291
  1.70    0.51179    0.70459    0.71175    0.72154    0.70226    0.67689    0.86166    0.86825    0.85515    0.98858
  1.80    0.45663    0.64067    0.64727    0.65623    0.63810    0.61411    0.79649    0.80281    0.79013    0.92604
  1.90    0.40756    0.58198    0.58802    0.59617    0.57930    0.55692    0.73494    0.74092    0.72884    0.86569
  2.00    0.36401    0.52838    0.53387    0.54125    0.52569    0.50498    0.67722    0.68282    0.67144    0.80787

  2.50    0.21047    0.32653    0.32987    0.33427    0.32442    0.31123    0.44561    0.44936    0.44159    0.56233
  3.00    0.12636    0.20559    0.20762    0.21028    0.20414    0.19590    0.29402    0.29644    0.29138    0.38787
  3.50    0.07901    0.13309    0.13437    0.13603    0.13211    0.12686    0.19717    0.19875    0.19543    0.26924
  4.00    0.05133    0.08875    0.08958    0.09066    0.08808    0.08463    0.13507    0.13612    0.13390    0.18949
  5.00    0.02395    0.04290    0.04328    0.04379    0.04257    0.04093    0.06776    0.06827    0.06719    0.09878
  6.00    0.01246    0.02281    0.02301    0.02327    0.02263    0.02178    0.03690    0.03717    0.03659    0.05515
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Atom	Na(1+)	Mg(2+)	Al(1+)	Al(3+)	Si(1+)	Si(2+)	Si(3+)	Si(4+)	Si(val)	P(1+)
Z	11	12	13	13	14	14	14	14	14	15
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	10.00000	10.00000	12.00000	10.00000	13.00000	12.00000	11.00000	10.00000	14.00000	14.00000
0.01	9.99528	9.99653	11.98733	9.99733	12.98523	11.99124	10.99495	9.99787	13.97401	13.98456
0.02	9.98115	9.98613	11.94962	9.98932	12.94126	11.96507	10.97983	9.99150	13.89701	13.93853
0.03	9.95767	9.96883	11.88776	9.97599	12.86906	11.92189	10.95481	9.98088	13.77188	13.86278
0.04	9.92495	9.94470	11.80315	9.95737	12.77021	11.86231	10.92013	9.96605	13.60312	13.75872
0.05	9.88314	9.91381	11.69769	9.93351	12.64680	11.78717	10.87613	9.94703	13.39654	13.62825
0.06	9.83245	9.87626	11.57364	9.90447	12.50136	11.69752	10.82323	9.92386	13.15881	13.47367
0.07	9.77311	9.83217	11.43353	9.87032	12.33675	11.59455	10.76191	9.89658	12.89700	13.29763
0.08	9.70538	9.78169	11.28004	9.83114	12.15600	11.47959	10.69274	9.86525	12.61818	13.10300
0.09	9.62957	9.72498	11.11591	9.78703	11.96226	11.35406	10.61631	9.82991	12.32905	12.89279
0.10	9.54602	9.66222	10.94382	9.73809	11.75865	11.21945	10.53326	9.79065	12.03567	12.67008
0.11	9.45509	9.59361	10.76631	9.68443	11.54817	11.07725	10.44424	9.74752	11.74324	12.43788
0.12	9.35717	9.51935	10.58572	9.62619	11.33362	10.92893	10.34992	9.70062	11.45608	12.19913
0.13	9.25266	9.43967	10.40411	9.56350	11.11755	10.77592	10.25096	9.65002	11.17755	11.95654
0.14	9.14199	9.35481	10.22326	9.49649	10.90219	10.61959	10.14802	9.59583	10.91013	11.71265
0.15	9.02560	9.26502	10.04462	9.42534	10.68946	10.46117	10.04171	9.53813	10.65550	11.46968
0.16	8.90393	9.17057	9.86933	9.35018	10.48094	10.30182	9.93262	9.47703	10.41461	11.22962
0.17	8.77744	9.07171	9.69826	9.27120	10.27787	10.14255	9.82132	9.41263	10.18786	10.99412
0.18	8.64659	8.96872	9.53196	9.18856	10.08119	9.98424	9.70829	9.34506	9.97516	10.76454
0.19	8.51184	8.86189	9.37079	9.10243	9.89155	9.82764	9.59400	9.27442	9.77608	10.54198
0.20	8.37363	8.75149	9.21486	9.01301	9.70933	9.67334	9.47887	9.20084	9.58991	10.32723
0.22	8.08865	8.52113	8.91842	8.82500	9.36764	9.37349	9.24740	9.04535	9.25272	9.92322
0.24	7.79511	8.27994	8.64085	8.62605	9.05536	9.08711	9.01615	8.87960	8.95556	9.55447
0.25	7.64616	8.15599	8.50824	8.52294	8.90946	8.94928	8.90111	8.79321	8.81939	9.38318
0.26	7.49627	8.03017	8.37919	8.41767	8.76980	8.81502	8.78663	8.70465	8.69015	9.22027
0.28	7.19515	7.77399	8.13011	8.20141	8.50718	8.55686	8.55974	8.52158	8.44882	8.91806
0.30	6.89447	7.51350	7.89042	7.97876	8.26339	8.31145	8.33590	8.33146	8.22501	8.64419
0.32	6.59661	7.25066	7.65742	7.75122	8.03442	8.07715	8.11517	8.13539	8.01338	8.39450
0.34	6.30368	6.98728	7.42900	7.52018	7.81667	7.85216	7.89743	7.93442	7.80978	8.16480
0.35	6.15962	6.85592	7.31603	7.40378	7.71103	7.74259	7.78961	7.83242	7.70998	8.05620
0.36	6.01742	6.72503	7.20369	7.28701	7.60710	7.63471	7.68244	7.72959	7.61112	7.95113
0.38	5.73930	6.46540	6.98058	7.05296	7.40332	7.42322	7.46993	7.52192	7.41523	7.74992
0.40	5.47049	6.20971	6.75922	6.81922	7.20348	7.21637	7.25968	7.31237	7.22071	7.55814
0.42	5.21190	5.95911	6.53956	6.58688	7.00632	7.01313	7.05154	7.10185	7.02671	7.37330
0.44	4.96418	5.71458	6.32180	6.35691	6.81101	6.81275	6.84545	6.89124	6.83286	7.19340
0.45	4.84454	5.59485	6.21376	6.24311	6.71389	6.71349	6.74318	6.78615	6.73597	7.10481
0.46	4.72778	5.47694	6.10635	6.13022	6.61709	6.61478	6.64145	6.68134	6.63913	7.01693
0.48	4.50298	5.24685	5.89371	5.90757	6.42440	6.41896	6.43966	6.47289	6.44570	6.84279
0.50	4.28986	5.02486	5.68444	5.68966	6.23303	6.22526	6.24029	6.26659	6.25295	6.67026
0.55	3.80772	4.50753	5.17970	5.16922	5.76201	5.75112	5.75420	5.76412	5.77717	6.24350
0.60	3.39486	4.04608	4.70744	4.68854	5.30638	5.29489	5.28965	5.28670	5.31663	5.82288
0.65	3.04540	3.64023	4.27329	4.25125	4.87253	4.86168	4.85149	4.83998	4.87878	5.41149
0.70	2.75217	3.28736	3.88025	3.85851	4.46589	4.45618	4.44364	4.42743	4.46935	5.01415
0.80	2.30468	2.72337	3.21853	3.20226	3.74747	3.74015	3.72784	3.71025	3.74849	4.27977
0.90	1.99700	2.31483	2.70978	2.70037	3.16165	3.15615	3.14699	3.13331	3.16275	3.64565
1.00	1.78454	2.02252	2.32859	2.32477	2.69992	2.69568	2.69012	2.68151	2.70197	3.11962
1.10	1.63451	1.81329	2.04703	2.04697	2.34430	2.34095	2.33838	2.33416	2.34727	2.69606
1.20	1.52414	1.66145	1.83984	1.84190	2.07418	2.07151	2.07104	2.06999	2.07770	2.36205
1.30	1.43820	1.54814	1.68631	1.68928	1.87012	1.86799	1.86883	1.86976	1.87377	2.10217
1.40	1.36688	1.46005	1.57047	1.57353	1.71550	1.71385	1.71534	1.71730	1.71892	1.90128
1.50	1.30403	1.38806	1.48045	1.48310	1.59696	1.59572	1.59741	1.59972	1.59992	1.74595
1.60	1.24596	1.32610	1.40773	1.40972	1.50417	1.50331	1.50489	1.50710	1.50652	1.62497
1.70	1.19055	1.27025	1.34636	1.34758	1.42941	1.42887	1.43017	1.43201	1.43109	1.52938
1.80	1.13671	1.21804	1.29226	1.29269	1.36702	1.36676	1.36768	1.36902	1.36803	1.45221
1.90	1.08392	1.16803	1.24272	1.24242	1.31296	1.31294	1.31346	1.31422	1.31334	1.38818
2.00	1.03205	1.11938	1.19600	1.19505	1.26441	1.26459	1.26470	1.26491	1.26421	1.33337
2.50	0.79042	0.88964	0.97989	0.97707	1.05591	1.05665	1.05534	1.05351	1.05392	1.12236
3.00	0.59074	0.68867	0.78338	0.78031	0.86750	0.86834	0.86658	0.86411	0.86507	0.94270
3.50	0.43753	0.52552	0.61498	0.61228	0.69892	0.69967	0.69799	0.69561	0.69667	0.77753
4.00	0.32439	0.39940	0.47868	0.47649	0.55649	0.55710	0.55566	0.55363	0.55460	0.63242
5.00	0.18250	0.23327	0.29000	0.28867	0.34939	0.34977	0.34884	0.34752	0.34819	0.41101
6.00	0.10725	0.14069	0.17948	0.17867	0.22187	0.22211	0.22152	0.22070	0.22113	0.26773

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Atom      P(2+)      P(3+)      P(4+)      P(5+)      S(1+)      S(2+)      S(3+)      S(4+)      S(5+)      S(6+)
   Z         15         15         15         15         16         16         16         16         16         16
Method       DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
  0.00  13.00000   12.00000   11.00000   10.00000   15.00000   14.00000   13.00000   12.00000   11.00000   10.00000
  0.01  12.98965   11.99344   10.99608    9.99826   14.98452   13.98886   12.99220   11.99486   10.99685    9.99856
  0.02  12.95874   11.97384   10.98434    9.99306   14.93832   13.95559   12.96886   11.97947   10.98742    9.99423
  0.03  12.90771   11.94138   10.96488    9.98440   14.86215   13.90060   12.93023   11.95395   10.97176    9.98702
  0.04  12.83727   11.89640   10.93782    9.97229   14.75719   13.82458   12.87669   11.91850   10.94995    9.97694
  0.05  12.74839   11.83935   10.90336    9.95676   14.62508   13.72846   12.80876   11.87337   10.92211    9.96400

  0.06  12.64226   11.77077   10.86175    9.93782   14.46780   13.61340   12.72709   11.81890   10.88840    9.94822
  0.07  12.52028   11.69134   10.81326    9.91550   14.28766   13.48076   12.63246   11.75549   10.84899    9.92962
  0.08  12.38398   11.60180   10.75823    9.88985   14.08721   13.33206   12.52576   11.68358   10.80409    9.90822
  0.09  12.23504   11.50295   10.69700    9.86917   13.86917   13.16895   12.40794   11.60369   10.75391    9.88404
  0.10  12.07519   11.39567   10.62997    9.82867   13.63634   12.99317   12.28004   11.51634   10.69873    9.85713

  0.11  11.90621   11.28086   10.55755    9.79325   13.39156   12.80654   12.14314   11.42213   10.63879    9.82751
  0.12  11.72985   11.15945   10.48016    9.75467   13.13763   12.61087   11.99836   11.32165   10.57438    9.79521
  0.13  11.54785   11.03238   10.39823    9.71298   12.87726   12.40797   11.84682   11.21553   10.50581    9.76028
  0.14  11.36187   10.90057   10.31221    9.66826   12.61300   12.19962   11.68967   11.10440   10.43336    9.72276
  0.15  11.17345   10.76493   10.22254    9.62057   12.34721   11.98750   11.52800   10.98890   10.35734    9.68270

  0.16  10.98404   10.62633   10.12964    9.56997   12.08207   11.77322   11.36289   10.86964   10.27807    9.64014
  0.17  10.79494   10.48558   10.03392    9.51655   11.81948   11.55826   11.19536   10.74725   10.19585    9.59514
  0.18  10.60730   10.34345    9.93580    9.46036   11.56113   11.34398   11.02638   10.62232   10.11097    9.54775
  0.19  10.42212   10.20066    9.83565    9.40151   11.30842   11.13160   10.85685   10.49542   10.02375    9.49802
  0.20  10.24023   10.05784    9.73383    9.34006   11.06253   10.92218   10.68760   10.36710    9.93445    9.44601

  0.22   9.88899    9.77433    9.52648    9.20973   10.59476   10.51581   10.35285   10.10817    9.75075    9.33540
  0.24   9.55739    9.49662    9.31608    9.07008   10.16269   10.13051   10.02707    9.84915    9.56189    9.21644
  0.25   9.39959    9.36078    9.21034    8.99699    9.96074    9.94692    9.86874    9.72054    9.46610    9.15399
  0.26   9.24723    9.22728    9.10452    8.92186    9.76824    9.76974    9.71391    9.59297    9.36967    9.08966
  0.28   8.95866    8.96790    8.89322    8.76583    9.41096    9.43507    9.41575    9.34193    9.17559    8.95560
  0.30   8.69063    8.71918    8.68324    8.60278    9.08877    9.12654    9.13382    9.09766    8.98090    8.81486

  0.32   8.44130    8.48110    8.47524    8.43350    8.79847    8.84301    8.86845    8.86121    8.78658    8.66801
  0.34   8.20834    8.25318    8.26962    8.25879    8.53628    8.58253    8.61919    8.63311    8.59334    8.51566
  0.35   8.09722    8.14276    8.16777    8.16965    8.41448    8.46019    8.50031    8.52223    8.49729    8.43761
  0.36   7.98927    8.03455    8.06656    8.07944    8.29820    8.34267    8.38506    8.41345    8.40170    8.35841
  0.38   7.78163    7.82416    7.86609    7.89623    8.08030    8.12074    8.16469    8.20201    8.21200    8.19685
  0.40   7.58317    7.62090    7.66814    7.70992    7.87889    7.91402    7.95654    7.99831    8.02444    8.03159

  0.42   7.39188    7.42368    7.47257    7.52125    7.69067    7.71993    7.75896    7.80172    7.83908    7.86322
  0.44   7.20609    7.23149    7.27927    7.33095    7.51272    7.53606    7.57034    7.61150    7.65593    7.69232
  0.45   7.11482    7.13700    7.18344    7.23540    7.42683    7.44729    7.47891    7.51856    7.56518    7.60609
  0.46   7.02444    7.04346    7.08813    7.13970    7.34263    7.36031    7.38917    7.42692    7.47496    7.51944
  0.48   6.84590    6.85889    6.89906    6.94815    7.17836    7.19086    7.21410    7.24724    7.29610    7.34513
  0.50   6.66973    6.67722    6.71204    6.75691    7.01831    7.02623    7.04393    7.07179    7.11927    7.16993

  0.55   6.23682    6.23350    6.25373    6.28386    6.62923    6.62839    6.63393    6.64795    6.68578    6.73120
  0.60   5.81326    5.80321    5.81005    5.82412    6.24786    6.24173    6.23837    6.24028    6.26445    6.29706
  0.65   5.40095    5.38927    5.38380    5.38393    5.87065    5.86181    5.85272    5.84556    5.85606    5.87356
  0.70   5.00380    4.98890    4.97821    4.96792    5.49874    5.48885    5.47656    5.46339    5.46230    5.46566
  0.80   4.27112    4.25702    4.24032    4.21974    4.78459    4.77514    4.76118    4.74295    4.72728    4.71084
  0.90   3.63886    3.62712    3.61132    3.59043    4.13417    4.12628    4.11356    4.09556    4.07532    4.05114
  1.00   3.11432    3.10498    3.09294    3.07642    3.56689    3.56055    3.54986    3.53414    3.51539    3.49181

  1.10   2.69186    2.68452    2.67676    2.66579    3.08906    3.08398    3.07528    3.06229    3.04772    3.02880
  1.20   2.35868    2.35294    2.34888    2.34289    2.69706    2.69296    2.68598    2.67552    2.66568    2.65257
  1.30   2.09945    2.09498    2.09367    2.09146    2.38157    2.37823    2.37267    2.36439    2.35875    2.35099
  1.40   1.89910    1.89564    1.89615    1.89649    2.13091    2.12819    2.12377    2.11730    2.11493    2.11143
  1.50   1.74423    1.74160    1.74315    1.74498    1.93317    1.93097    1.92750    1.92249    1.92242    1.92194

  1.60   1.62366    1.62172    1.62372    1.62623    1.77745    1.77569    1.77300    1.76919    1.77055    1.77200
  1.70   1.52842    1.52705    1.52910    1.53173    1.65431    1.65294    1.65091    1.64807    1.65019    1.65268
  1.80   1.45156    1.45067    1.45249    1.45488    1.55599    1.55496    1.55347    1.55144    1.55380    1.55668
  1.90   1.38781    1.38732    1.38875    1.39067    1.47623    1.47550    1.47448    1.47310    1.47536    1.47817
  2.00   1.33323    1.33308    1.33406    1.33538    1.41016    1.40969    1.40906    1.40822    1.41016    1.41259

  2.50   1.12293    1.12372    1.12257    1.12110    1.18252    1.18290    1.18343    1.18413    1.18355    1.18288
  3.00   0.94347    0.94449    0.94237    0.93959    1.00936    1.01006    1.01097    1.01212    1.00990    1.00716
  3.50   0.77828    0.77925    0.77696    0.77397    0.84979    0.85053    0.85147    0.85264    0.84989    0.84646
  4.00   0.63306    0.63388    0.63181    0.62909    0.70501    0.70568    0.70652    0.70754    0.70487    0.70151
  5.00   0.41143    0.41196    0.41053    0.40864    0.47364    0.47410    0.47467    0.47536    0.47336    0.47086
  6.00   0.26799    0.26833    0.26739    0.26617    0.31633    0.31663    0.31700    0.31745    0.31610    0.31440
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---------------------------------------------- Page   5 ----------------------------------------------------------
Atom    Cl(1+)    Cl(2+)    Cl(3+)    Cl(4+)    Cl(5+)    Cl(6+)    Cl(7+)    Cl(1-)    K(1+)     Ca(2+)
   Z       17        17        17        17        17        17        17        17        19        20
Method    DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF
  STL
 0.00   16.00000  15.00000  14.00000  13.00000  12.00000  11.00000  10.00000  18.00000  18.00000  18.00000
 0.01   15.98478  14.98852  13.99146  12.99385  11.99584  10.99741   9.99878  17.97178  17.98566  17.98868
 0.02   15.93933  14.95422  13.96592  12.97544  11.98337  10.98963   9.99512  17.88786  17.94277  17.95480
 0.03   15.86425  14.89746  13.92361  12.94492  11.96268  10.97672   9.98902  17.75045  17.87177  17.89861
 0.04   15.76056  14.81888  13.86492  12.90251  11.93388  10.95872   9.98050  17.56306  17.77336  17.82054
 0.05   15.62963  14.71931  13.79037  12.84853  11.89714  10.93571   9.96955  17.33027  17.64851  17.72117

 0.06   15.47314  14.59982  13.70063  12.78337  11.85268  10.90778   9.95620  17.05744  17.49844  17.60121
 0.07   15.29306  14.46165  13.59647  12.70750  11.80075  10.87506   9.94045  16.75044  17.32458  17.46155
 0.08   15.09161  14.30621  13.47879  12.62147  11.74163  10.83769   9.92232  16.41538  17.12855  17.30318
 0.09   14.87116  14.13504  13.34858  12.52587  11.67566  10.79580   9.90183  16.05828  16.91212  17.12720
 0.10   14.63421  13.94979  13.20689  12.42136  11.60320  10.74958   9.87900  15.68498  16.67722  16.93483

 0.11   14.38332  13.75217  13.05486  12.30864  11.52463  10.69921   9.85386  15.30089  16.42585  16.72736
 0.12   14.12108  13.54394  12.89364  12.18844  11.44036  10.64487   9.82643  14.91094  16.16006  16.50613
 0.13   13.85001  13.32687  12.72443  12.06151  11.35082  10.58678   9.79674  14.51948  15.88197  16.27257
 0.14   13.57259  13.10272  12.54843  11.92862  11.25644  10.52514   9.76483  14.13031  15.59366  16.02809
 0.15   13.29115  12.87319  12.36683  11.79055  11.15768  10.46018   9.73071  13.74663  15.29719  15.77415

 0.16   13.00788  12.63995  12.18079  11.64808  11.05499  10.39211   9.69443  13.37110  14.99458  15.51221
 0.17   12.72481  12.40455  11.99146  11.50196  10.94881  10.32116   9.65603  13.00586  14.68775  15.24370
 0.18   12.44376  12.16846  11.79992  11.35293  10.83961  10.24756   9.61554  12.65259  14.37854  14.97001
 0.19   12.16635  11.93303  11.60719  11.20172  10.72781  10.17153   9.57301  12.31254  14.06866  14.69253
 0.20   11.89401  11.69948  11.41424  11.04901  10.61386  10.09329   9.52847  11.98659  13.75971  14.41256

 0.22   11.36915  11.24231  11.03112  10.74162  10.38111   9.93107   9.43355  11.37904  13.15028  13.85007
 0.24   10.87647  10.80414  10.65669  10.43541  10.14444   9.76254   9.33117  10.83146  12.56020  13.29168
 0.25   10.64366  10.59385  10.47427  10.28399  10.02551   9.67640   9.27730  10.57976  12.27490  13.01652
 0.26   10.42032  10.39007  10.29573  10.13427   9.90660   9.58926   9.22171  10.34230  11.99714  12.74521
 0.28   10.00257  10.00326   9.95170   9.84130   9.66992   9.41260   9.10559   9.90798  11.46657  12.21710
 0.30    9.62309   9.64521   9.62683   9.55879   9.43632   9.23379   8.98323   9.52369  10.97197  11.71239

 0.32    9.28027   9.31600   9.32224   9.28828   9.20729   9.05385   8.85508   9.18400  10.51508  11.23476
 0.34    8.97146   9.01461   9.03813   9.03064   8.98392   8.87365   8.72159   8.88327  10.09622  10.78665
 0.35    8.82879   8.87383   8.90360   8.90675   8.87460   8.78367   8.65299   8.74580   9.90081  10.57411
 0.36    8.69335   8.73928   8.77394   8.78614   8.76693   8.69387   8.58323   8.61602   9.71452  10.36938
 0.38    8.44236   8.48768   8.52855   8.55461   8.55672   8.51505   8.44045   8.37703   9.36828   9.98331
 0.40    8.21479   8.25722   8.30048   8.33547   8.35339   8.33758   8.29374   8.16153   9.05517   9.62803

 0.42    8.00708   8.04517   8.08797   8.12788   8.15685   8.16173   8.14354   7.96527   8.77245   9.30246
 0.44    7.81590   7.84886   7.88918   7.93084   7.96680   7.98768   7.99033   7.78448   8.51720   9.00507
 0.45    7.72554   7.75580   7.79434   7.83593   7.87409   7.90136   7.91274   7.69886   8.39892   8.86637
 0.46    7.63820   7.66575   7.70224   7.74323   7.78285   7.81553   7.83456   7.61594   8.28638   8.73398
 0.48    7.47132   7.49350   7.52535   7.56390   7.60452   7.64530   7.67668   7.45688   8.07702   8.48706
 0.50    7.31294   7.33003   7.35686   7.39175   7.43128   7.47701   7.51713   7.30504   7.88625   8.26210

 0.55    6.94213   6.94849   6.96291   6.98602   7.01703   7.06453   7.11370   6.94555   7.47358   7.78089
 0.60    6.59113   6.58999   6.59404   6.60503   6.62387   6.66339   6.70864   6.60030   7.12515   7.38903
 0.65    6.24812   6.24231   6.23880   6.23955   6.24628   6.27336   6.30752   6.25942   6.81447   7.05756
 0.70    5.90834   5.90000   5.89152   5.88461   5.88111   5.89486   5.91509   5.91968   6.52357   6.76392
 0.80    5.23935   5.22971   5.21690   5.20164   5.18511   5.17700   5.17142   5.24821   5.96220   6.23068
 0.90    4.60189   4.59317   4.58015   4.56280   4.54141   4.52147   4.50000   4.60790   5.40575   5.71853
 1.00    4.01900   4.01171   4.00008   3.98368   3.96225   3.93904   3.91191   4.02299   4.85827   5.20930

 1.10    3.50577   3.49981   3.48997   3.47567   3.45641   3.43520   3.40939   3.50857   4.33589   4.70920
 1.20    3.06751   3.06265   3.05453   3.04256   3.02620   3.00943   2.98846   3.06970   3.85386   4.23168
 1.30    2.70205   2.69807   2.69143   2.68165   2.66819   2.65642   2.64137   2.70395   3.42211   3.78907
 1.40    2.40261   2.39934   2.39396   2.38608   2.37524   2.36803   2.35855   2.40436   3.04476   3.38957
 1.50    2.16029   2.15760   2.15327   2.14699   2.13840   2.13486   2.12997   2.16193   2.72139   3.03691

 1.60    1.96567   1.96346   1.96001   1.95507   1.94835   1.94751   1.94605   1.96719   2.44845   2.73117
 1.70    1.80982   1.80804   1.80532   1.80148   1.79632   1.79728   1.79814   1.81120   2.22068   2.46987
 1.80    1.68481   1.68340   1.68130   1.67838   1.67448   1.67651   1.67877   1.68601   2.03209   2.24897
 1.90    1.58389   1.58280   1.58123   1.57907   1.57622   1.57873   1.58166   1.58490   1.87664   2.06369
 2.00    1.50150   1.50069   1.49956   1.49804   1.49604   1.49862   1.50170   1.50230   1.74869   1.90907

 2.50    1.24044   1.24060   1.24085   1.24118   1.24159   1.24191   1.24235   1.24032   1.36712   1.44389
 3.00    1.06876   1.06934   1.07012   1.07110   1.07230   1.07034   1.06800   1.06812   1.17406   1.22538
 3.50    0.91537   0.91607   0.91697   0.91807   0.91941   0.91640   0.91278   0.91456   1.02804   1.07766
 4.00    0.77323   0.77390   0.77475   0.77578   0.77700   0.77381   0.76994   0.77243   0.89451   0.94815
 5.00    0.53615   0.53664   0.53725   0.53798   0.53884   0.53625   0.53310   0.53554   0.65697   0.71434
 6.00    0.36695   0.36728   0.36769   0.36817   0.36874   0.36691   0.36468   0.36653   0.47122   0.52388
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Atom      Sc(1+)     Sc(2+)     Sc(3+)     Ti(2+)     Ti(3+)     Ti(4+)     V(1+)      V(2+)      V(3+)      V(4+)
   Z         21         21         21         22         22         22         23         23         23         23
Method      DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
  STL
  0.00    20.00000   19.00000   18.00000   20.00000   19.00000   18.00000   22.00000   21.00000   20.00000   19.00000
  0.01    19.97761   18.98806   17.99077   19.98784   18.99048   17.99229   21.98359   20.98783   19.99034   18.99210
  0.02    19.91112   18.95233   17.96313   19.95147   18.96196   17.96921   21.93457   20.95141   19.96140   18.96844
  0.03    19.80250   18.89311   17.91724   19.89118   18.91462   17.93087   21.85358   20.89102   19.91336   18.92912
  0.04    19.65486   18.81090   17.85337   19.80747   18.84874   17.87744   21.74166   20.80714   19.84649   18.87433
  0.05    19.47221   18.70637   17.77190   19.70102   18.76470   17.80918   21.60022   20.70042   19.76117   18.80433

  0.06    19.25914   18.58037   17.67329   19.57266   18.66299   17.72642   21.43096   20.57165   19.65788   18.71943
  0.07    19.02054   18.43388   17.55812   19.42341   18.54420   17.62955   21.23584   20.42180   19.53720   18.62002
  0.08    18.76128   18.26805   17.42704   19.25438   18.40900   17.51900   21.01698   20.25194   19.39979   18.50655
  0.09    18.48596   18.08410   17.28078   19.06682   18.25814   17.39529   20.77666   20.06327   19.24639   18.37953
  0.10    18.19875   17.88337   17.12014   18.86206   18.09246   17.25899   20.51717   19.85707   19.07782   18.23951

  0.11    17.90324   17.66726   16.94601   18.64151   17.91283   17.11070   20.24083   19.63469   18.89494   18.08711
  0.12    17.60240   17.43722   16.75930   18.40660   17.72021   16.95107   19.94993   19.39752   18.69869   17.92297
  0.13    17.29858   17.19473   16.56098   18.15881   17.51556   16.78081   19.64665   19.14701   18.49003   17.74778
  0.14    16.99359   16.94127   16.35207   17.89963   17.29992   16.60063   19.33308   18.88459   18.26996   17.56227
  0.15    16.68872   16.67833   16.13359   17.63052   17.07433   16.41129   19.01117   18.61170   18.03951   17.36718

  0.16    16.38491   16.40736   15.90660   17.35294   16.83982   16.21355   18.68274   18.32975   17.79971   17.16328
  0.17    16.08276   16.12979   15.67215   17.06830   16.59748   16.00821   18.34948   18.04013   17.55159   16.95134
  0.18    15.78269   15.84700   15.43131   16.77796   16.34833   15.79607   18.01289   17.74417   17.29621   16.73217
  0.19    15.48498   15.56030   15.18512   16.48322   16.09344   15.57793   17.67437   17.44317   17.03459   16.50655
  0.20    15.18984   15.27096   14.93460   16.18533   15.83382   15.35457   17.33516   17.13836   16.76772   16.27529

  0.22    14.60799   14.68902   14.42461   15.58471   15.30435   14.89542   16.65908   16.52187   16.22219   15.79896
  0.24    14.03878   14.10978   13.90897   14.98459   14.76746   14.42479   15.99226   15.90316   15.66707   15.30932
  0.25    13.75955   13.82353   13.65123   14.68703   14.49842   14.18701   15.66426   15.59531   15.38809   15.06135
  0.26    13.48431   13.54062   13.39463   14.39224   14.23005   13.94853   15.34074   15.28955   15.10923   14.81222
  0.28    12.94709   12.98762   12.88776   13.81374   13.69822   13.47208   14.70924   14.68720   14.55477   14.31310
  0.30    12.42984   12.45566   12.39363   13.25400   13.17727   13.00031   14.10139   14.10117   14.00906   13.81690

  0.32    11.93515   11.94841   11.91658   12.71686   12.67163   12.53755   13.51990   13.53549   13.47662   13.32802
  0.34    11.46527   11.46853   11.46004   12.20516   12.18486   12.08746   12.96669   12.99326   12.96120   12.85025
  0.35    11.24017   11.23941   11.24030   11.95950   11.94945   11.86815   12.70111   12.73168   12.71084   12.61657
  0.36    11.02187   11.01768   11.02657   11.72088   11.71974   11.65310   12.44303   12.47675   12.46579   12.38683
  0.38    10.60606   10.59670   10.61788   11.26522   11.27826   11.23686   11.94960   11.98747   11.99265   11.94034
  0.40    10.21832   10.20570   10.23496   10.83869   10.86172   10.84056   11.48659   11.52630   11.54339   11.51286

  0.42     9.85853    9.84419    9.87812   10.44125   10.47083   10.46543   11.05376   11.09358   11.11901   11.10586
  0.44     9.52610    9.51121    9.54714   10.07239   10.10571   10.11220   10.65051   10.68916   10.72001   10.72036
  0.45     9.36984    9.35502    9.39115    9.89840    9.93274    9.94389   10.45970   10.49741   10.53005   10.53586
  0.46     9.22001    9.20543    9.24132    9.73119    9.76607    9.78112   10.27594   10.31252   10.34642   10.35691
  0.48     8.93889    8.92522    8.95961    9.41647    9.45122    9.47207    9.92891    9.96281    9.99789   10.01567
  0.50     8.68117    8.66879    8.70066    9.12678    9.16017    9.18455    9.60810    9.63893    9.67377    9.69645

  0.55     8.12746    8.11899    8.14249    8.50141    8.52828    8.55452    8.91088    8.93353    8.96376    8.99097
  0.60     7.67994    7.67520    7.69031    7.99555    8.01451    8.03704    8.34321    8.35825    8.38130    8.40633
  0.65     7.31091    7.30908    7.31770    7.58246    7.59438    7.61145    7.87967    7.88853    7.90436    7.92440
  0.70     6.99650    6.99661    7.00119    7.23795    7.24468    7.25675    7.49659    7.50094    7.51077    7.52542
  0.80     6.46054    6.46213    6.46493    6.67777    6.67994    6.68656    6.89260    6.89242    6.89532    6.90241
  0.90     5.97542    5.97662    5.98238    6.20189    6.20495    6.21197    6.40825    6.40762    6.40929    6.41443
  1.00     5.50099    5.50118    5.51098    5.75258    5.75878    5.76915    5.97205    5.97288    5.97644    5.98341

  1.10     5.02976    5.02901    5.04197    5.30881    5.31821    5.33234    5.55043    5.55318    5.55956    5.56976
  1.20     4.56889    4.56752    4.58214    4.86945    4.88112    4.89799    5.13313    5.13751    5.14639    5.15960
  1.30     4.12946    4.12782    4.14271    4.44181    4.45459    4.47275    4.72202    4.72748    4.73802    4.75323
  1.40     3.72125    3.71962    3.73375    4.03502    4.04787    4.06600    4.32381    4.32978    4.34105    4.35711
  1.50     3.35082    3.34936    3.36209    3.65678    3.66894    3.68605    3.94586    3.95188    3.96310    3.97900

  1.60     3.02126    3.02008    3.03110    3.31221    3.32321    3.33867    3.59420    3.59993    3.61055    3.62553
  1.70     2.73282    2.73194    2.74118    3.00375    3.01336    3.02685    3.27281    3.27804    3.28769    3.30128
  1.80     2.48368    2.48309    2.49063    2.73163    2.73979    2.75123    2.98359    2.98821    2.99671    3.00866
  1.90     2.27068    2.27034    2.27635    2.49443    2.50119    2.51066    2.72670    2.73067    2.73796    2.74821
  2.00     2.08997    2.08983    2.09451    2.28961    2.29509    2.30275    2.50097    2.50432    2.51044    2.51902

  2.50     1.53304    1.53329    1.53415    1.63700    1.63837    1.64027    1.75465    1.75570    1.75761    1.76026
  3.00     1.27931    1.27942    1.27925    1.33836    1.33838    1.33839    1.40412    1.40426    1.40451    1.40485
  3.50     1.12480    1.12470    1.12443    1.17066    1.17042    1.17008    1.21736    1.21726    1.21708    1.21682
  4.00     0.99779    0.99755    0.99738    1.04344    1.04324    1.04299    1.08692    1.08680    1.08660    1.08632
  5.00     0.76907    0.76876    0.76878    0.82004    0.82002    0.82002    0.86815    0.86811    0.86807    0.86802
  6.00     0.57611    0.57584    0.57593    0.62665    0.62671    0.62682    0.67589    0.67590    0.67595    0.67603
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Atom      V(5+)     Cr(1+)     Cr(2+)     Cr(3+)     Cr(4+)     Cr(5+)     Cr(6+)     Mn(1+)     Mn(2+)     Mn(3+)
    Z        23         24         24         24         24         24         24         25         25         25
Method      DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
  0.00   18.00000   23.00000   22.00000   21.00000   20.00000   19.00000   18.00000   24.00000   23.00000   22.00000
  0.01   17.99345   22.98407   21.98792   20.99029   19.99199   18.99330   17.99436   23.98050   22.98808   21.99031
  0.02   17.97384   22.93645   21.95178   20.96123   19.96799   18.97322   17.97745   23.92239   22.95239   21.96131
  0.03   17.94123   22.85772   21.89183   20.91296   19.92811   18.93984   17.94933   23.82683   22.89319   21.91314
  0.04   17.89576   22.74877   21.80852   20.84577   19.87253   18.89328   17.91010   23.69565   22.81087   21.84604
  0.05   17.83761   22.61084   21.70245   20.76000   19.80149   18.83373   17.85989   23.53127   22.70600   21.76038

  0.06   17.76701   22.44544   21.57437   20.65612   19.71531   18.76140   17.79885   23.33657   22.57928   21.65658
  0.07   17.68423   22.25430   21.42519   20.53469   19.61437   18.67658   17.72721   23.11474   22.43153   21.53517
  0.08   17.58959   22.03935   21.25591   20.39634   19.49910   18.57957   17.64519   22.86911   22.26371   21.39676
  0.09   17.48346   21.80262   21.06766   20.24179   19.36999   18.47074   17.55307   22.60304   22.07685   21.24202
  0.10   17.36625   21.54624   20.86165   20.07182   19.22760   18.35048   17.45113   22.31978   21.87210   21.07170

  0.11   17.23840   21.27235   20.63917   19.88727   19.07251   18.21922   17.33972   22.02239   21.65067   20.88660
  0.12   17.10037   20.98309   20.40153   19.68903   18.90536   18.07745   17.21918   21.71365   21.41379   20.68757
  0.13   16.95269   20.68054   20.15012   19.47804   18.72681   17.92565   17.08990   21.39605   21.16278   20.47551
  0.14   16.79587   20.36672   19.88630   19.25528   18.53759   17.76436   16.95228   21.07174   20.89893   20.25135
  0.15   16.63050   20.04352   19.61147   19.02172   18.33841   17.59412   16.80674   20.74256   20.62357   20.01604

  0.16   16.45713   19.71273   19.32699   18.77837   18.13002   17.41551   16.65372   20.41003   20.33802   19.77054
  0.17   16.27637   19.37604   19.03421   18.52626   17.91320   17.22911   16.49369   20.07544   20.04356   19.51584
  0.18   16.08882   19.03498   18.73443   18.26638   17.68871   17.03552   16.32710   19.73981   19.74147   19.25290
  0.19   15.89510   18.69096   18.42891   17.99974   17.45735   16.83536   16.15444   19.40399   19.43296   18.98271
  0.20   15.69583   18.34527   18.11886   17.72733   17.21988   16.62924   15.97619   19.06866   19.11922   18.70622

  0.22   15.28315   17.65342   17.48972   17.16902   16.72974   16.20159   15.60491   18.40168   18.48050   18.13808
  0.24   14.85573   16.96743   16.85543   16.59880   16.22436   15.75750   15.21724   17.74245   17.83367   17.55570
  0.25   14.63800   16.62869   16.53870   16.31138   15.96778   15.53079   15.01848   17.41664   17.50955   17.26129
  0.26   14.41837   16.29371   16.22335   16.02348   15.70955   15.30176   14.81709   17.09378   17.18609   16.96580
  0.28   13.97569   15.63734   15.59974   15.44917   15.19073   14.83900   14.40832   16.45811   16.54411   16.37447
  0.30   13.53197   15.00224   14.98983   14.88128   14.67288   14.37354   13.99461   15.83770   15.91311   15.78716

  0.32   13.09118   14.39143   14.39788   14.32446   14.16046   13.90941   13.57942   15.23471   15.29754   15.20862
  0.34   12.65683   13.80711   13.82722   13.78263   13.65740   13.45023   13.16599   14.65112   14.70099   14.64290
  0.35   12.44306   13.52540   13.55070   13.51835   13.41044   13.22352   12.96085   14.36717   14.41075   14.36592
  0.36   12.23204   13.25083   13.28041   13.25896   13.16704   12.99922   12.75722   14.08871   14.12626   14.09336
  0.38   11.81943   12.72356   12.75927   12.75598   12.69221   12.55918   12.35574   13.54899   13.57545   13.56274
  0.40   11.42121   12.22577   12.26500   12.27555   12.23514   12.13247   11.96383   13.03317   13.05007   13.05315

  0.42   11.03910   11.75755   11.79827   11.81899   11.79760   11.72102   11.58343   12.54213   12.55109   12.56618
  0.44   10.67443   11.31859   11.35928   11.38709   11.38083   11.32638   11.21616   12.07641   12.07900   12.10289
  0.45   10.49892   11.10991   11.15013   11.18051   11.18051   11.13572   11.03786   11.85314   11.85309   11.88035
  0.46   10.32808   10.90830   10.94782   10.98020   10.98567   10.94965   10.86329   11.63627   11.63392   11.66393
  0.48   10.00061   10.52585   10.56338   10.59829   10.61253   10.59162   10.52580   11.22164   11.21563   11.24954
  0.50    9.69221   10.17020   10.20519   10.24100   10.26152   10.25273   10.20435   10.83221   10.82362   10.85964

  0.55    9.00344    9.39011    9.41755    9.45081    9.47869    9.48948    9.47298    9.96482    9.95339    9.98914
  0.60    8.42508    8.74826    8.76799    8.79509    8.82258    8.84177    8.84380    9.23781    9.22684    9.25770
  0.65    7.94349    8.22153    8.23452    8.25454    8.27783    8.29861    8.30993    8.63363    8.62469    8.64892
  0.70    7.54215    7.78736    7.79501    7.80854    7.82643    7.84525    7.86007    8.13295    8.12654    8.14410
  0.80    6.91365    7.11702    7.11828    7.12297    7.13175    7.14410    7.15822    7.36695    7.36490    7.37218
  0.90    6.42377    6.60677    6.60605    6.60748    6.61214    6.62059    6.63264    6.80757    6.80791    6.81008
  1.00    5.99445    6.17236    6.17214    6.17401    6.17879    6.18714    6.19945    6.35929    6.36027    6.36135

  1.10    5.58413    5.76743    5.76872    5.77270    5.77979    5.79044    5.80509    5.96252    5.96308    5.96532
  1.20    5.17718    5.37161    5.37451    5.38088    5.39080    5.40446    5.42217    5.58544    5.58515    5.58940
  1.30    4.77300    4.98001    4.98420    4.99250    5.00477    5.02100    5.04136    5.21480    5.21362    5.21984
  1.40    4.37775    4.59555    4.60056    4.61008    4.62381    4.64165    4.66365    4.84824    4.84637    4.85409
  1.50    3.99931    4.22412    4.22949    4.23950    4.25378    4.27215    4.29461    4.48889    4.48658    4.49519

  1.60    3.64462    3.87174    3.87712    3.88702    3.90106    3.91904    3.94092    4.14183    4.13932    4.14826
  1.70    3.31857    3.54329    3.54841    3.55777    3.57100    3.58789    3.60841    3.81214    3.80965    3.81845
  1.80    3.02386    3.24198    3.24668    3.25522    3.26727    3.28262    3.30126    3.50394    3.50161    3.50993
  1.90    2.76123    2.96939    2.97357    2.98115    2.99182    3.00541    3.02189    3.21996    3.21789    3.22551
  2.00    2.52994    2.72568    2.72932    2.73588    2.74511    2.75686    2.77111    2.96163    2.95986    2.96667

  2.50    1.76362    1.88778    1.88914    1.89157    1.89496    1.89927    1.90448    2.03664    2.03623    2.03916
  3.00    1.40527    1.47845    1.47874    1.47926    1.47998    1.48088    1.48196    1.56279    1.56292    1.56374
  3.50    1.21651    1.26622    1.26617    1.26608    1.26595    1.26579    1.26560    1.31877    1.31891    1.31894
  4.00    1.08599    1.12886    1.12875    1.12856    1.12830    1.12797    1.12759    1.17047    1.17047    1.17031
  5.00    0.86797    0.91315    0.91310    0.91302    0.91294    0.91284    0.91273    0.95548    0.95525    0.95515
  6.00    0.67614    0.72329    0.72330    0.72332    0.72337    0.72345    0.72354    0.76891    0.76862    0.76863
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Atom    Mn(4+)    Mn(5+)    Mn(6+)    Mn(7+)    Fe(1+)    Fe(2+)    Fe(3+)    Fe(4+)    Fe(5+)    Fe(6+)
   Z       25        25        25        25        26        26        26        26        26        26
Method    DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF
   STL
  0.00  21.00000  20.00000  19.00000  18.00000  25.00000  24.00000  23.00000  22.00000  21.00000  20.00000
  0.01  20.99194  19.99320  18.99422  17.99508  24.98118  23.98827  22.99038  21.99192  20.99314  19.99413
  0.02  20.96778  19.97282  18.97691  17.98034  24.92507  23.95315  22.96156  21.96773  20.97257  19.97653
  0.03  20.92763  19.93893  18.94812  17.95581  24.83269  23.89486  22.91369  21.92752  20.93838  19.94726
  0.04  20.87166  19.89166  18.90795  17.92158  24.70568  23.81379  22.84700  21.87145  20.89068  19.90641
  0.05  20.80010  19.83118  18.85651  17.87773  24.54621  23.71044  22.76181  21.79975  20.82963  19.85410

  0.06  20.71326  19.75770  18.79399  17.82439  24.35688  23.58547  22.65855  21.71271  20.75545  19.79050
  0.07  20.61151  19.67150  18.72056  17.76172  24.14056  23.43963  22.53769  21.61066  20.66838  19.71578
  0.08  20.49525  19.57288  18.63648  17.68990  23.90030  23.27381  22.39982  21.49402  20.56872  19.63019
  0.09  20.36496  19.46218  18.54199  17.60913  23.63919  23.08899  22.24557  21.36323  20.45682  19.53397
  0.10  20.22118  19.33980  18.43740  17.51962  23.36025  22.88621  22.07565  21.21880  20.33304  19.42741

  0.11  20.06447  19.20616  18.32302  17.42165  23.06636  22.66661  21.89082  21.06127  20.19778  19.31082
  0.12  19.89543  19.06171  18.19920  17.31547  22.76017  22.43135  21.69188  20.89123  20.05149  19.18454
  0.13  19.71474  18.90693  18.06633  17.20137  22.44408  22.18167  21.47969  20.70929  19.89465  19.04894
  0.14  19.52305  18.74236  17.92478  17.07967  22.12020  21.91880  21.25513  20.51612  19.72774  18.90439
  0.15  19.32108  18.56851  17.77498  16.95069  21.79037  21.64399  21.01910  20.31239  19.55128  18.75131

  0.16  19.10956  18.38594  17.61737  16.81477  21.45616  21.35849  20.77254  20.09880  19.36582  18.59011
  0.17  18.88922  18.19524  17.45238  16.67227  21.11887  21.06355  20.51639  19.87607  19.17191  18.42124
  0.18  18.66083  17.99699  17.28049  16.52355  20.77963  20.76038  20.25157  19.64492  18.97012  18.24515
  0.19  18.42514  17.79179  17.10216  16.36899  20.43932  20.45017  19.97903  19.40610  18.76103  18.06230
  0.20  18.18292  17.58023  16.91788  16.20898  20.09873  20.13406  19.69970  19.16033  18.54524  17.87316

  0.22  17.68190  17.14051  16.53343  15.87418  19.41909  19.48851  19.12430  18.65093  18.09591  17.47794
  0.24  17.16372  16.68267  16.13105  15.52232  18.74478  18.83196  18.53240  18.12253  17.62686  17.06336
  0.25  16.89999  16.44845  15.92436  15.34100  18.41062  18.50189  18.23235  17.85297  17.38642  16.85002
  0.26  16.63410  16.21147  15.71466  15.15662  18.07892  18.17174  17.93061  17.58074  17.14280  16.63329
  0.28  16.09844  15.73150  15.28811  14.78026  17.42419  17.51426  17.32497  17.03089  16.64824  16.19154
  0.30  15.56172  15.24711  14.85511  14.39637  16.78298  16.86502  16.72095  16.47793  16.14751  15.74182

  0.32  15.02844  14.76234  14.41916  14.00794  16.15754  16.22862  16.12335  15.92640  15.64468  15.28764
  0.34  14.50261  14.28089  13.98354  13.61782  15.54991  15.60885  15.53634  15.38036  15.14346  14.83233
  0.35  14.24361  14.04246  13.76681  13.42295  15.25337  15.30619  15.24793  15.11053  14.89454  14.60522
  0.36  13.98773  13.80608  13.55128  13.22865  14.96195  15.00877  14.96344  14.84339  14.64726  14.37896
  0.38  13.48674  13.34082  13.12508  12.84289  14.39528  14.43073  14.40757  14.31859  14.15909  13.93033
  0.40  13.00210  12.88763  12.70737  12.46275  13.85123  13.87650  13.87107  13.80857  13.68158  13.48895

  0.42  12.53578  12.44863  12.30023  12.09020  13.33083  13.34732  13.35574  13.31548  13.21701  13.05704
  0.44  12.08925  12.02553  11.90544  11.72695  12.83482  12.84398  12.86291  12.84102  12.76724  12.63651
  0.45  11.87376  11.82037  11.71314  11.54928  12.59612  12.60213  12.62523  12.61119  12.54840  12.43102
  0.46  11.66359  11.61966  11.52445  11.37446  12.36365  12.36686  12.39348  12.38646  12.33381  12.22896
  0.48  11.25949  11.23202  11.15841  11.03395  11.91747  11.91601  11.94796  11.95274  11.91788  11.83572
  0.50  10.87728  10.86325  10.80819  10.70638  11.49620  11.49120  11.52652  11.54040  11.52033  11.45782

  0.55  10.01708  10.02564  10.00513   9.94828  10.54937  10.53950  10.57700  10.60423  10.60983  10.58463
  0.60   9.28728   9.30659   9.30690   9.28068   9.74583   9.73497   9.76910   9.80019   9.81905   9.81712
  0.65   8.67541   8.69785   8.70914   8.70236   9.07083   9.06112   9.08933   9.11872   9.14251   9.15348
  0.70   8.16551   8.18675   8.20254   8.20708   8.50712   8.49949   8.52114   8.54608   8.56971   8.58649
  0.80   7.38352   7.39794   7.41322   7.42614   7.64275   7.63948   7.64988   7.66435   7.68141   7.69849
  0.90   6.81542   6.82426   6.83616   6.84983   7.02257   7.02220   7.02589   7.03282   7.04305   7.05586
  1.00   6.36504   6.37198   6.38245   6.39624   6.54559   6.54640   6.54749   6.55109   6.55774   6.56759

  1.10   5.97016   5.97811   5.98960   6.00486   6.14338   6.14417   6.14535   6.14878   6.15503   6.16448
  1.20   5.59655   5.60691   5.62083   5.63861   5.77509   5.77521   5.77781   5.78281   5.79059   5.80154
  1.30   5.22936   5.24230   5.25887   5.27935   5.41982   5.41910   5.42348   5.43059   5.44064   5.45389
  1.40   4.86544   4.88039   4.89906   4.92165   5.06964   5.06814   5.07412   5.08317   5.09537   5.11085
  1.50   4.50761   4.52373   4.54359   4.56732   4.72405   4.72198   4.72912   4.73959   4.75335   4.77048

  1.60   4.16102   4.17745   4.19753   4.22138   4.38620   4.38379   4.39160   4.40285   4.41746   4.43544
  1.70   3.83094   3.84694   3.86643   3.88949   4.06047   4.05792   4.06595   4.07739   4.09215   4.11020
  1.80   3.52169   3.53673   3.55501   3.57659   3.75105   3.74855   3.75642   3.76758   3.78191   3.79937
  1.90   3.23626   3.24999   3.26665   3.28630   3.46131   3.45898   3.46643   3.47695   3.49042   3.50680
  2.00   2.97625   2.98847   3.00329   3.02077   3.19351   3.19143   3.19828   3.20794   3.22027   3.23525

  2.50   2.04324   2.04843   2.05472   2.06212   2.19593   2.19526   2.19862   2.20332   2.20930   2.21654
  3.00   1.56486   1.56629   1.56801   1.57004   1.65734   1.65738   1.65850   1.66007   1.66205   1.66444
  3.50   1.31898   1.31903   1.31909   1.31917   1.37666   1.37681   1.37699   1.37724   1.37754   1.37791
  4.00   1.17008   1.16980   1.16947   1.16909   1.21309   1.21314   1.21302   1.21286   1.21266   1.21243
  5.00   0.95503   0.95489   0.95473   0.95454   0.99514   0.99495   0.99484   0.99469   0.99452   0.99432
  6.00   0.76865   0.76869   0.76874   0.76881   0.81205   0.81177   0.81176   0.81175   0.81175   0.81177
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----------------------------------------------- Page   9 -----------------------------------------------
Atom    Co(1+)    Co(2+)    Co(3+)    Co(4+)    Co(5+)    Ni(1+)    Ni(2+)    Ni(3+)    Ni(4+)    Cu(1+)
   Z        27        27        27        27        27        28        28        28        28        29
Method     DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF
  STL
  0.00  26.00000  25.00000  24.00000  23.00000  22.00000  27.00000  26.00000  25.00000  24.00000  28.00000
  0.01  25.98546  24.98848  23.99047  22.99194  21.99311  26.98589  25.98870  24.99058  23.99199  27.98630
  0.02  25.94199  24.95398  23.96192  22.96781  21.97246  26.94369  25.95486  24.96236  23.96798  27.94531
  0.03  25.86995  24.89672  23.91450  22.92769  21.93812  26.87373  25.89866  24.91548  23.92806  27.87733
  0.04  25.76999  24.81703  23.84840  22.87174  21.89019  26.77659  25.82044  24.85012  23.87238  27.78289
  0.05  25.64298  24.71540  23.76396  22.80017  21.82885  26.65305  25.72062  24.76658  23.80114  27.66268

  0.06  25.48997  24.59241  23.66154  22.71325  21.75429  26.50405  25.59975  24.66522  23.71459  27.51757
  0.07  25.31223  24.44877  23.54161  22.61131  21.66675  26.33075  25.45850  24.54648  23.61305  27.34858
  0.08  25.11115  24.28531  23.40470  22.49473  21.56652  26.13441  25.29760  24.41084  23.49687  27.15690
  0.09  24.88828  24.10292  23.25143  22.36394  21.45391  25.91643  25.11789  24.25889  23.36647  26.94377
  0.10  24.64521  23.90258  23.08245  22.21942  21.32929  25.67829  24.92030  24.09124  23.22229  26.71058

  0.11  24.38365  23.68534  22.89848  22.06169  21.19304  25.42153  24.70580  23.90856  23.06482  26.45873
  0.12  24.10528  23.45232  22.70028  21.89130  21.04558  25.14774  24.47542  23.71159  22.89460  26.18971
  0.13  23.81183  23.20464  22.48866  21.70884  20.88738  24.85852  24.23023  23.50107  22.71219  25.90500
  0.14  23.50499  22.94348  22.26445  21.51495  20.71890  24.55546  23.97134  23.27780  22.51818  25.60609
  0.15  23.18643  22.67003  22.02853  21.31027  20.54064  24.24013  23.69985  23.04260  22.31319  25.29446

  0.16  22.85773  22.38547  21.78177  21.09547  20.35313  23.91404  23.41690  22.79632  22.09787  24.97155
  0.17  22.52045  22.09098  21.52506  20.87124  20.15690  23.57868  23.12361  22.53979  21.87287  24.63878
  0.18  22.17602  21.78774  21.25932  20.63828  19.95250  23.23544  22.82109  22.27389  21.63886  24.29750
  0.19  21.82583  21.47688  20.98544  20.39730  19.74050  22.88567  22.51045  21.99947  21.39653  23.94969
  0.20  21.47116  21.15951  20.70431  20.14901  19.52147  22.53062  22.19275  21.71740  21.14656  23.59448

  0.22  20.75307  20.50950  20.12382  19.63336  19.06462  21.80932  21.54028  21.13369  20.62645  22.87203
  0.24  20.03024  19.84575  19.52472  19.09697  18.58658  21.08002  20.87152  20.52939  20.08400  22.13853
  0.25  19.66933  19.51103  19.22022  18.82272  18.34104  20.71467  20.53331  20.22150  19.80608  21.76996
  0.26  19.30982  19.17553  18.91346  18.54533  18.09192  20.34994  20.19364  19.91079  19.52457  21.40126
  0.28  18.59769  18.50525  18.29601  17.98369  17.58511  19.62516  19.51301  19.28379  18.95326  20.66636
  0.30  17.89869  17.84048  17.67782  17.41694  17.07043  18.91070  18.83525  18.65375  18.37493  19.93902

  0.32  17.21668  17.18596  17.06372  16.84961  16.55191  18.21064  18.16520  18.02555  17.79407  19.22352
  0.34  16.55472  16.54567  16.45797  16.28579  16.03331  17.52829  17.50696  17.40348  17.21478  18.52337
  0.35  16.23202  16.23190  16.15939  16.00637  15.77506  17.19459  17.18336  17.09594  16.92690  18.17995
  0.36  15.91518  15.92285  15.86422  15.72916  15.51806  16.86625  16.86394  16.79129  16.64077  17.84138
  0.38  15.29985  15.32008  15.28553  15.18289  15.00924  16.22657  16.23894  16.19217  16.07532  17.17980
  0.40  14.71002  14.73938  14.72444  14.64975  14.50961  15.61074  15.63417  15.60881  15.52127  16.54036

  0.42  14.14654  14.18224  14.18295  14.13203  14.02153  15.01987  15.05135  15.04340  14.98107  15.92437
  0.44  13.60991  13.64968  13.66262  13.63161  13.54704  14.45467  14.49173  14.49768  14.45674  15.33275
  0.45  13.35174  13.39284  13.41076  13.38836  13.31542  14.18183  14.22091  14.23264  14.20107  15.04628
  0.46  13.10032  13.14236  13.16457  13.14997  13.08780  13.91555  13.95620  13.97299  13.94995  14.76611
  0.48  12.61768  12.66057  12.68955  12.68823  12.64518  13.40264  13.44526  13.47027  13.46197  14.22478
  0.50  12.16167  12.20432  12.23797  12.24718  12.22021  12.91583  12.95917  12.99017  12.99379  13.70885

  0.55  11.13453  11.17336  11.21178  11.23745  11.23927  11.81067  11.85193  11.89042  11.91364  12.52901
  0.60  10.25861  10.29123  10.32801  10.35991  10.37762  10.85758  10.89363  10.93237  10.96431  11.50076
  0.65   9.51842   9.54420   9.57604   9.60784   9.63245  10.04358  10.07321  10.10818  10.14180  10.61350
  0.70   8.89665   8.91592   8.94155   8.96979   8.99555   9.35331   9.37646   9.40581   9.43697   9.85389
  0.80   7.93816   7.94713   7.96099   7.97888   7.99888   8.27907   8.29124   8.30871   8.33012   8.65838
  0.90   7.25336   7.25615   7.26197   7.27117   7.28352   7.51048   7.51538   7.52377   7.53572   7.79674
  1.00   6.73863   6.73859   6.74039   6.74474   6.75204   6.94271   6.94371   6.94680   6.95258   7.16496

  1.10   6.32030   6.31963   6.32038   6.32322   6.32869   6.49700   6.49650   6.49741   6.50038   6.68097
  1.20   5.95115   5.95101   5.95245   5.95593   5.96190   6.11942   6.11887   6.11964   6.12224   6.28546
  1.30   5.60416   5.60504   5.60790   5.61303   5.62070   5.77631   5.77645   5.77815   5.78176   5.93889
  1.40   5.26630   5.26824   5.27263   5.27960   5.28929   5.44894   5.45002   5.45305   5.45823   5.61710
  1.50   4.93329   4.93612   4.94181   4.95036   4.96180   5.12870   5.13068   5.13501   5.14176   5.30701

  1.60   4.60582   4.60929   4.61589   4.62554   4.63820   4.81323   4.81595   4.82132   4.82935   5.00292
  1.70   4.28689   4.29074   4.29784   4.30806   4.32132   4.50365   4.50689   4.51297   4.52185   4.70365
  1.80   3.98017   3.98416   3.99140   4.00171   4.01502   4.20269   4.20622   4.21268   4.22198   4.41053
  1.90   3.68907   3.69303   3.70010   3.71013   3.72302   3.91347   3.91710   3.92365   3.93298   4.12596
  2.00   3.41629   3.42006   3.42676   3.43623   3.44836   3.63883   3.64242   3.64881   3.65787   3.85262

  2.50   2.36191   2.36405   2.36778   2.37299   2.37963   2.53786   2.54018   2.54418   2.54979   2.71867
  3.00   1.76135   1.76219   1.76363   1.76564   1.76818   1.87596   1.87699   1.87873   1.88116   1.99980
  3.50   1.44072   1.44093   1.44128   1.44176   1.44236   1.51170   1.51202   1.51256   1.51329   1.59011
  4.00   1.25791   1.25788   1.25783   1.25777   1.25768   1.30570   1.30572   1.30576   1.30581   1.35747
  5.00   1.03276   1.03268   1.03256   1.03240   1.03221   1.06908   1.06900   1.06888   1.06872   1.10459
  6.00   0.85275   0.85272   0.85269   0.85266   0.85263   0.89158   0.89155   0.89150   0.89145   0.92843
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Atom    Cu(2+)    Cu(3+)    Cu(4+)    Zn(2+)    Ga(1+)    Ga(2+)    Ga(3+)    Ge(1+)    Ge(2+)    Ge(3+)
   Z       29        29        29        30        31        31        31        32        32        32
Method     DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF
   STL
  0.00   27.00000  26.00000  25.00000  28.00000  30.00000  29.00000  28.00000  31.00000  30.00000  29.00000
  0.01   26.98892  25.99070  24.99205  27.98915  29.98169  28.98698  27.99097  30.97903  29.98541  28.98919
  0.02   26.95575  25.96286  24.96821  27.95664  29.92702  28.94803  27.96392  30.91649  29.94177  28.95685
  0.03   26.90065  25.91657  24.92858  27.90263  29.83682  28.88350  27.91895  30.81348  29.86955  28.90319
  0.04   26.82392  25.85204  24.87329  27.82741  29.71241  28.79398  27.85623  30.67179  29.76946  28.82855
  0.05   26.72597  25.76953  24.80253  27.73133  29.55557  28.68025  27.77598  30.49378  29.64251  28.73344

  0.06   26.60729  25.66938  24.71654  27.61487  29.36846  28.54326  27.67851  30.28232  29.48992  28.61846
  0.07   26.46850  25.55199  24.61561  27.47859  29.15353  28.38417  27.56417  30.04064  29.31313  28.48432
  0.08   26.31029  25.41784  24.50009  27.32312  28.91345  28.20421  27.43337  29.77220  29.11374  28.33184
  0.09   26.13343  25.26745  24.37035  27.14921  28.65100  28.00477  27.28657  29.48059  28.89348  28.16193
  0.10   25.93879  25.10141  24.22683  26.95762  28.36900  27.78726  27.12430  29.16937  28.65417  27.97553

  0.11   25.72726  24.92036  24.06999  26.74922  28.07020  27.55315  26.94711  28.84202  28.39766  27.77367
  0.12   25.49982  24.72496  23.90034  26.52491  27.75726  27.30394  26.75560  28.50178  28.12584  27.55740
  0.13   25.25746  24.51595  23.71841  26.28561  27.43268  27.04108  26.55041  28.15168  27.84055  27.32778
  0.14   25.00122  24.29406  23.52476  26.03232  27.09873  26.76602  26.33221  27.79440  27.54358  27.08588
  0.15   24.73215  24.06007  23.31998  25.76601  26.75746  26.48012  26.10169  27.43231  27.23666  26.83276

  0.16   24.45133  23.81479  23.10469  25.48771  26.41069  26.18469  25.85957  27.06744  26.92140  26.56948
  0.17   24.15981  23.55902  22.87951  25.19841  26.05998  25.88098  25.60658  26.70149  26.59929  26.29704
  0.18   23.85866  23.29358  22.64508  24.89914  25.70667  25.57012  25.34347  26.33584  26.27170  26.01643
  0.19   23.54894  23.01930  22.40206  24.59088  25.35186  25.25318  25.07099  25.97157  25.93988  25.72857
  0.20   23.23165  22.73700  22.15111  24.27464  24.99645  24.93112  24.78988  25.60953  25.60492  25.43435

  0.22   22.57840  22.15161  21.62806  23.62201  24.28665  24.27510  24.20483  24.89435  24.92938  24.83012
  0.24   21.90653  21.54383  21.08121  22.94863  23.58144  23.60818  23.59425  24.19309  24.25139  24.20975
  0.25   21.56583  21.23346  20.80049  22.60631  23.23137  23.27223  23.28120  23.84797  23.91296  23.89517
  0.26   21.22305  20.91977  20.51575  22.26133  22.88329  22.93534  22.96390  23.50651  23.57553  23.57843
  0.28   20.53428  20.28520  19.93668  21.56637  22.19366  22.26066  22.31927  22.83421  22.90499  22.94057
  0.30   19.84584  19.64544  19.34876  20.86932  21.51345  21.58750  21.66549  22.17527  22.24191  22.29988

  0.32   19.16262  19.00532  18.75642  20.17512  20.84335  20.91870  21.00730  21.52866  21.58772  21.65952
  0.34   18.48885  18.36918  18.16378  19.48805  20.18406  20.25672  20.34901  20.89356  20.94339  21.02214
  0.35   18.15664  18.05381  17.86852  19.14835  19.85869  19.92898  20.02106  20.58014  20.62515  20.70531
  0.36   17.82807  17.74082  17.57455  18.81177  19.53632  19.60372  19.69450  20.26942  20.30964  20.39007
  0.38   17.18323  17.12355  16.99206  18.14937  18.90102  18.96164  19.04720  19.65605  19.68708  19.76530
  0.40   16.55675  16.52017  16.41926  17.50342  18.27912  18.33220  18.41010  19.05357  19.07633  19.14960

  0.42   15.95052  15.93304  15.85868  16.87600  17.67161  17.71698  17.78578  18.46236  18.47799  18.54457
  0.44   15.36601  15.36405  15.31249  16.26874  17.07951  17.11736  17.17641  17.88303  17.89271  17.95160
  0.45   15.08225  15.08686  15.04537  15.97308  16.78955  16.82379  16.87791  17.59804  17.60519  17.66004
  0.46   14.80430  14.81473  14.78249  15.68291  16.50379  16.53455  16.58379  17.31630  17.32119  17.37196
  0.48   14.26613  14.28622  14.27012  15.11943  15.94534  15.96960  16.00940  16.76297  16.76411  16.80678
  0.50   13.75193  13.77934  13.77652  14.57894  15.40495  15.42337  15.45437  16.22384  16.22216  16.25703

  0.55   12.57194  12.60963  12.62952  13.33005  14.13691  14.14378  14.15657  14.94318  14.93752  14.95540
  0.60   11.53966  11.57962  11.61079  12.22654  12.99192  12.99122  12.99156  13.76609  13.75938  13.76470
  0.65   10.64661  10.68541  10.71891  11.26237  11.97111  11.96605  11.95901  12.69856  12.69230  12.68936
  0.70    9.88072   9.91342   9.94701  10.42758  11.07105  11.06397  11.05342  11.74207  11.73690  11.72925
  0.80    8.67385   8.69493   8.71980   9.09589   9.60296   9.59603   9.58537  10.14916  10.14644  10.13646
  0.90    7.80404   7.81531   7.83031   8.12510   8.50945   8.50492   8.49791   8.93556   8.93463   8.92701
  1.00    7.16737   7.17224   7.17997   7.41408   7.70192   7.69987   7.69669   8.02712   8.02718   8.02299

  1.10    6.68102   6.68262   6.68633   6.87858   7.09869   7.09837   7.09788   7.34750   7.34796   7.34661
  1.20    6.28483   6.28541   6.28772   6.45446   6.63275   6.63330   6.63418   6.82938   6.82986   6.83026
  1.30    5.93854   5.93946   5.94205   6.09645   6.25362   6.25436   6.25555   6.41893   6.41923   6.42036
  1.40    5.61747   5.61940   5.62314   5.77488   5.92590   5.92637   5.92718   6.07619   6.07622   6.07731
  1.50    5.30822   5.31134   5.31650   5.47191   5.62650   5.62647   5.62655   5.77342   5.77316   5.77376

  1.60    5.00490   5.00910   5.01558   5.17811   5.34165   5.34105   5.34029   5.49268   5.49215   5.49205
  1.70    4.70624   4.71129   4.71880   4.88958   5.06415   5.06302   5.06148   5.22340   5.22264   5.22179
  1.80    4.41353   4.41914   4.42732   4.60582   4.79119   4.78963   4.78745   4.96015   4.95920   4.95769
  1.90    4.12920   4.13510   4.14358   4.32818   4.52259   4.52073   4.51809   4.70094   4.69985   4.69781
  2.00    3.85594   3.86188   3.87036   4.05881   4.25968   4.25764   4.25472   4.44587   4.44468   4.44228

  2.50    2.72110   2.72529   2.73116   2.90433   3.09591   3.09425   3.09186   3.28557   3.28435   3.28200
  3.00    2.00099   2.00303   2.00585   2.13314   2.27631   2.27561   2.27463   2.42644   2.42553   2.42441
  3.50    1.59055   1.59129   1.59230   1.67670   1.77170   1.77160   1.77148   1.87540   1.87483   1.87460
  4.00    1.35756   1.35770   1.35789   1.41411   1.47604   1.47614   1.47631   1.54459   1.54428   1.54441
  5.00    1.10452   1.10440   1.10425   1.13987   1.17558   1.17559   1.17560   1.21233   1.21233   1.21239
  6.00    0.92838   0.92833   0.92825   0.96345   0.99733   0.99717   0.99693   1.02953   1.02964   1.02945
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Atom	Ge(4+)	As(2+)	As(3+)	As(5+)	Se(2+)	Se(4+)	Se(6+)	Br(1+)	Br(3+)	Br(4+)
Z	32	33	33	33	34	34	34	35	35	35
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	28.00000	31.00000	30.00000	28.00000	32.00000	30.00000	28.00000	34.00000	32.00000	31.00000
0.01	27.99228	30.98344	29.98785	27.99328	31.98219	29.98961	27.99408	33.97672	31.98517	30.98829
0.02	27.96915	30.93394	29.95147	27.97315	31.92896	29.95849	27.97632	33.90721	31.94080	30.95324
0.03	27.93068	30.85210	29.89117	27.93964	31.84095	29.90684	27.94676	33.79245	31.86730	30.89511
0.04	27.87698	30.73887	29.80739	27.89285	31.71918	29.83498	27.90546	33.63404	31.76532	30.81428
0.05	27.80821	30.59555	29.70076	27.83289	31.56505	29.74333	27.85252	33.43416	31.63576	30.71133
0.06	27.72458	30.42375	29.57208	27.75991	31.38030	29.63244	27.78803	33.19547	31.47974	30.58695
0.07	27.62632	30.22534	29.42229	27.67407	31.16693	29.50295	27.71214	32.92106	31.29858	30.44196
0.08	27.51372	30.00237	29.25242	27.57560	30.92721	29.35561	27.62500	32.61435	31.09379	30.27733
0.09	27.38711	29.75707	29.06365	27.46473	30.66354	29.19125	27.52678	32.27898	30.86700	30.09409
0.10	27.24685	29.49176	28.85722	27.34172	30.37847	29.01074	27.41770	31.91874	30.61998	29.89338
0.11	27.09332	29.20879	28.63444	27.20686	30.07462	28.81504	27.29797	31.53745	30.35455	29.67640
0.12	26.92697	28.91053	28.39665	27.06047	29.75458	28.60515	27.16783	31.13890	30.07263	29.44441
0.13	26.74824	28.59926	28.14521	26.90288	29.42093	28.38209	27.02754	30.72675	29.77612	29.19869
0.14	26.55761	28.27718	27.88149	26.73446	29.07615	28.14690	26.87738	30.30450	29.46693	28.94056
0.15	26.35560	27.94638	27.60683	26.55559	28.72259	27.90063	26.71765	29.87538	29.14692	28.67130
0.16	26.14272	27.60879	27.32256	26.36667	28.36245	27.64433	26.54864	29.44236	28.81792	28.39221
0.17	25.91952	27.26615	27.02992	26.16810	27.99775	27.37903	26.37068	29.00812	28.48166	28.10455
0.18	25.68656	26.92005	26.73012	25.96032	27.63032	27.10573	26.18411	28.57500	28.13976	27.80954
0.19	25.44441	26.57187	26.42430	25.74377	27.26178	26.82540	25.98928	28.14501	27.79376	27.50835
0.20	25.19364	26.22283	26.11351	25.51890	26.89354	26.53897	25.78654	27.71986	27.44505	27.20207
0.22	24.66863	25.52605	25.48082	25.04604	26.16257	25.95129	25.35879	26.88935	26.74446	26.57834
0.24	24.11623	24.83595	24.83885	24.54549	25.44477	25.34914	24.90390	26.09124	26.04658	25.94576
0.25	23.83123	24.49471	24.51615	24.28602	25.09232	25.04441	24.66723	25.70569	25.70075	25.62812
0.26	23.54113	24.15648	24.19309	24.02106	24.74470	24.73806	24.42493	25.32944	25.35787	25.31046
0.28	22.94792	23.48979	23.54780	23.47653	24.06469	24.12271	23.92503	24.60482	24.68286	24.67732
0.30	22.34103	22.83677	22.90620	22.91563	23.40536	23.50685	23.40731	23.91611	24.02439	24.05004
0.32	21.72469	22.19744	22.27064	22.34201	22.76616	22.89348	22.87488	23.26061	23.38388	23.43128
0.34	21.10285	21.57139	21.64281	21.75917	22.14581	22.28491	22.33075	22.63490	22.76170	22.82280
0.35	20.79104	21.26315	21.33218	21.46534	21.84221	21.98299	22.05522	22.33204	22.45737	22.52277
0.36	20.47922	20.95799	21.02391	21.17043	21.54271	21.68289	21.77787	22.03522	22.15744	22.22565
0.38	19.85716	20.35663	20.41483	20.57893	20.95514	21.08873	21.21904	21.45793	21.57019	21.64035
0.40	19.23974	19.76684	19.81621	19.98759	20.38156	20.50340	20.65694	20.89965	20.99881	21.06702
0.42	18.62971	19.18832	19.22862	19.39909	19.82062	19.92763	20.09408	20.35747	20.44202	20.50553
0.44	18.02948	18.62100	18.65255	18.81589	19.27127	19.36201	19.53280	19.82896	19.89863	19.95564
0.45	17.73372	18.34156	18.36898	18.52697	19.00070	19.08316	19.25345	19.56921	19.63161	19.68496
0.46	17.44117	18.06498	18.08848	18.24019	18.73278	18.80701	18.97528	19.31221	19.36755	19.41705
0.48	16.86658	17.52053	17.53690	17.67395	18.20472	18.26304	18.42350	18.80579	18.84790	18.88948
0.50	16.30723	16.98808	16.99832	17.11890	17.68691	17.73050	17.87924	18.30872	18.33900	18.37270
0.55	14.98317	15.71273	15.71194	15.78948	16.43791	16.45164	16.56155	17.10377	17.11119	17.12725
0.60	13.77468	14.52384	14.51715	14.55620	15.25809	15.25241	15.32045	15.95234	15.94583	15.94877
0.65	12.68704	13.42868	13.41968	13.42903	14.15814	14.13814	14.16930	14.84921	14.84558	14.84014
0.70	11.71962	12.43179	12.42264	12.41184	13.13338	13.11287	13.11565	13.83152	13.81538	13.80543
0.80	10.12270	10.73457	10.72793	10.70017	11.35417	11.33553	11.30783	11.99722	11.98317	11.97165
0.90	8.91627	9.40747	9.40393	9.37807	9.92302	9.91099	9.87839	10.47683	10.46784	10.45919
1.00	8.01701	8.39508	8.39384	8.37687	8.80646	8.80063	8.77557	9.26044	9.25603	9.25098
1.10	7.34462	7.63071	7.63082	7.62301	7.95118	7.94963	7.93534	8.31125	8.31000	8.30787
1.20	6.83077	7.04996	7.05064	7.04953	7.29877	7.29959	7.29458	7.57998	7.58051	7.58027
1.30	6.42192	6.59777	6.59850	6.60109	6.79513	6.79686	6.79797	7.01596	7.01723	7.01796
1.40	6.07888	6.23083	6.23132	6.23508	6.39502	6.39667	6.40076	6.57366	6.57498	6.57600
1.50	5.77468	5.91736	5.91745	5.92063	6.06330	6.06432	6.06892	6.21565	6.21660	6.21748
1.60	5.49204	5.63541	5.63507	5.63666	5.77436	5.77447	5.77795	5.91313	5.91351	5.91400
1.70	5.22078	5.37091	5.37015	5.36974	5.51063	5.50976	5.51124	5.64524	5.64498	5.64495
1.80	4.95578	5.11562	5.11449	5.11207	5.26090	5.25909	5.25826	5.39772	5.39684	5.39628
1.90	4.69518	4.86540	4.86397	4.85978	5.01864	5.01602	5.01296	5.16152	5.16008	5.15902
2.00	4.43914	4.61884	4.61719	4.61161	4.78066	4.77739	4.77240	4.93142	4.92951	4.92802
2.50	3.27888	3.47209	3.47015	3.46324	3.65582	3.65134	3.64310	3.83490	3.83196	3.82948
3.00	2.42292	2.58181	2.58031	2.57652	2.74271	2.73902	2.73382	2.90762	2.90502	2.90283
3.50	1.87430	1.98678	1.98582	1.98477	2.10654	2.10408	2.10226	2.23417	2.23230	2.23077
4.00	1.54459	1.61957	1.61904	1.61929	1.70194	1.70051	1.70055	1.79198	1.79081	1.78988
5.00	1.21246	1.25086	1.25081	1.25110	1.29188	1.29166	1.29211	1.33613	1.33587	1.33567
6.00	1.02919	1.06090	1.06102	1.06059	1.09165	1.09188	1.09151	1.12228	1.12241	1.12251

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Atom    Br(5+)     Br(7+)     Br(1-)     Kr(2+)     Rb(1+)     Sr(2+)     Y(2+)      Y(3+)      Zr(1+)     Zr(2+)
   Z       35         35         35         36         37         38         39         39         40         40
Method     DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
 0.00   30.00000   28.00000   36.00000   34.00000   36.00000   36.00000   37.00000   36.00000   39.00000   38.00000
 0.01   29.99095   27.99472   35.96100   33.98095   35.97685   35.98062   36.97861   35.98336   38.96620   37.97764
 0.02   29.96386   27.97890   35.84510   33.92399   35.90769   35.92264   36.91469   35.93355   38.86573   37.91084
 0.03   29.91885   27.95256   35.65552   33.82972   35.79330   35.82659   36.80898   35.85093   38.70129   37.80038
 0.04   29.85616   27.91575   35.39734   33.69913   35.63501   35.69333   36.66269   35.73612   38.47714   37.64753
 0.05   29.77609   27.86853   35.07716   33.53356   35.43461   35.52404   36.47747   35.58994   38.19881   37.45405

 0.06   29.67904   27.81100   34.70262   33.33467   35.19432   35.32019   36.25532   35.41343   37.87270   37.22206
 0.07   29.56548   27.74326   34.28199   33.10443   34.91675   35.08353   35.99860   35.20783   37.50569   36.95405
 0.08   29.43595   27.66542   33.82369   32.84505   34.60482   34.81605   35.70988   34.97457   37.10474   36.65278
 0.09   29.29106   27.57763   33.33597   32.55894   34.26172   34.51994   35.39195   34.71523   36.67657   36.32120
 0.10   29.13147   27.48005   32.82661   32.24868   33.89079   34.19755   35.04771   34.43154   36.22736   35.96241

 0.11   28.95790   27.37283   32.30271   31.91692   33.49551   33.85137   34.68012   34.12533   35.76264   35.57955
 0.12   28.77108   27.25619   31.77059   31.56641   33.07938   33.48397   34.29216   33.79853   35.28715   35.17578
 0.13   28.57182   27.13030   31.23569   31.19986   32.64592   33.09795   33.88674   33.45314   34.80485   34.75421
 0.14   28.36092   26.99541   30.70263   30.81998   32.19854   32.69596   33.46671   33.09118   34.31893   34.31784
 0.15   28.13921   26.85172   30.17518   30.42937   31.74053   32.28059   33.03480   32.71471   33.83193   33.86956

 0.16   27.90751   26.69950   29.65636   30.03055   31.27501   31.85438   32.59358   32.32578   33.34578   33.41206
 0.17   27.66667   26.53899   29.14851   29.62587   30.80492   31.41980   32.14548   31.92639   32.86200   32.94789
 0.18   27.41750   26.37046   28.65334   29.21754   30.33293   30.97919   31.69275   31.51852   32.38170   32.47937
 0.19   27.16083   26.19419   28.17204   28.80757   29.86148   30.53476   31.23747   31.10407   31.90575   32.00865
 0.20   26.89745   26.01047   27.70535   28.39778   29.39274   30.08857   30.78152   30.68487   31.43482   31.53766

 0.22   26.35358   25.62184   26.81698   27.58502   28.47073   29.19834   29.87429   29.83899   30.51012   30.60158
 0.24   25.79169   25.20702   25.98780   26.78976   27.57897   28.32156   28.98264   28.99338   29.61114   29.68271
 0.25   25.50563   24.99057   25.59437   26.40111   27.14711   27.89152   28.54553   28.57405   29.17222   29.23258
 0.26   25.21697   24.76853   25.21421   26.01938   26.72557   27.46843   28.11546   28.15859   28.74079   28.78984
 0.28   24.63402   24.30897   24.49079   25.27846   25.91513   26.64634   27.27924   27.34312   27.90162   27.92925
 0.30   24.04674   23.83095   23.81132   24.56920   25.14941   25.86011   26.47831   26.55347   27.09576   27.10515

 0.32   23.45842   23.33709   23.16943   23.89192   24.42792   25.11233   25.71515   25.79417   26.32480   26.31995
 0.34   22.87177   22.83000   22.55909   23.24553   23.74855   24.40369   24.99069   25.06805   25.58963   25.57462
 0.35   22.57976   22.57228   22.26402   22.93331   23.42369   24.06385   24.64291   24.71788   25.23556   25.21687
 0.36   22.28893   22.31221   21.97484   22.62800   23.10810   23.73341   24.30459   24.37638   24.89044   24.86893
 0.38   21.71161   21.78623   21.41196   22.03674   22.50277   23.09964   23.65550   23.71921   24.22667   24.20175
 0.40   21.14113   21.25443   20.86650   21.46891   21.92847   22.49973   23.04137   23.09558   23.59714   23.57124

 0.42   20.57849   20.71912   20.33528   20.92165   21.38114   21.93063   22.45963   22.50378   23.00014   22.97504
 0.44   20.02449   20.18246   19.81583   20.39227   20.85696   21.38904   21.90741   21.94158   22.43355   22.41050
 0.45   19.75092   19.91427   19.55994   20.13352   20.60243   21.12754   21.64143   21.67079   22.16092   22.13921
 0.46   19.47972   19.64651   19.30636   19.87836   20.35241   20.87169   21.38171   21.40643   21.89499   21.87476
 0.48   18.94467   19.11317   18.80559   19.37785   19.86444   20.37542   20.87955   20.89566   21.38190   21.36492
 0.50   18.41974   18.58420   18.31276   18.88903   19.39042   19.89731   20.39805   20.40656   20.89171   20.87811

 0.55   17.15392   17.29117   17.11361   17.71019   18.25331   18.76527   19.26765   19.26195   19.75005   19.74436
 0.60   15.95837   16.05637   15.96347   16.58481   17.16857   17.70011   18.21554   18.20198   18.70054   18.70082
 0.65   14.83756   14.89532   14.86928   15.51035   16.12677   16.68336   17.21813   17.20156   17.71589   17.71988
 0.70   13.79541   13.81826   13.83955   14.48992   15.12712   15.70691   16.26203   16.24567   16.77791   16.78365
 0.80   11.95709   11.93500   12.00102   12.63273   13.27160   13.87460   14.45733   14.44574   15.00769   15.01317
 0.90   10.44723   10.41038   10.47776   11.04907   11.64343   12.22944   12.80869   12.80255   13.37155   13.37478
 1.00    9.24350    9.21021    9.25992    9.74783   10.26853   10.80352   11.34727   11.34491   11.89249   11.89354

 1.10    8.30434    8.28195    8.31025    8.70964    9.14528    9.60928   10.09455   10.09415   10.59612   10.59579
 1.20    7.57947    7.56855    7.57902    7.89722    8.25000    8.63690    9.05250    9.05278    9.49398    9.49305
 1.30    7.01866    7.01648    7.01526    7.26627    7.54681    7.86086    8.20585    8.20614    8.58093    8.57996
 1.40    6.57727    6.58039    6.57327    6.77339    6.99622    7.24786    7.52854    7.52860    7.83908    7.83835
 1.50    6.21867    6.22398    6.21555    6.38048    6.56088    6.76324    6.99000    6.98983    7.24328    7.24286

 1.60    5.91473    5.91990    5.91326    6.05658    6.20858    6.37504    6.55983    6.55954    6.76596    6.76583
 1.70    5.64504    5.64861    5.64555    5.77805    5.91342    6.05611    6.21065    6.21039    6.38060    6.38068
 1.80    5.39568    5.39689    5.39815    5.52780    5.65574    5.78477    5.91950    5.91939    6.06375    6.06393
 1.90    5.15776    5.15641    5.16204    5.29422    5.42138    5.54461    5.66815    5.66828    5.79588    5.79609
 2.00    4.92618    4.92242    4.93200    5.06992    5.20072    5.32384    5.44288    5.44329    5.56160    5.56176

 2.50    3.82627    3.81694    3.83557    4.00439    4.16766    4.31961    4.46007    4.46173    4.59117    4.59083
 3.00    2.90000    2.89324    2.90826    3.07181    3.23779    3.39971    3.55588    3.55774    3.70692    3.70639
 3.50    2.22881    2.22597    2.23470    2.36656    2.50581    2.64747    2.79007    2.79152    2.93358    2.93318
 4.00    1.78870    1.78836    1.79238    1.88818    1.99233    2.10176    2.21578    2.21671    2.33426    2.33407
 5.00    1.33543    1.33605    1.33625    1.38386    1.43610    1.49259    1.55361    1.55386    1.61938    1.61941
 6.00    1.12262    1.12238    1.12222    1.15342    1.18538    1.21870    1.25376    1.25378    1.29091    1.29094
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Atom      Zr(3+)     Zr(4+)     Nb(2+)     Nb(3+)     Nb(4+)     Nb(5+)     Mo(1+)     Mo(2+)     Mo(3+)     Mo(4+)
    Z        40         40         41         41         41         41         42         42         42         42
Method      DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
  0.00   37.00000   36.00000   39.00000   38.00000   37.00000   36.00000   41.00000   40.00000   39.00000   38.00000
  0.01   36.98213   35.98546   38.97721   37.98139   36.98456   35.98713   40.97157   39.97708   38.98096   37.98396
  0.02   36.92866   35.94193   38.90910   37.92571   36.93835   35.94860   40.88669   39.90857   38.92399   37.93595
  0.03   36.84005   35.86967   38.79643   37.83343   36.86167   35.88460   40.74663   39.79519   38.82955   37.85628
  0.04   36.71701   35.76913   38.64046   37.70532   36.75503   35.79546   40.55344   39.63811   38.69843   37.74548
  0.05   36.56055   35.64091   38.44289   37.54244   36.61912   35.68166   40.30985   39.43897   38.53166   37.60428

  0.06   36.37193   35.48578   38.20582   37.34611   36.45480   35.54377   40.01920   39.19974   38.33058   37.43360
  0.07   36.15261   35.30467   37.93170   37.11789   36.26313   35.38250   39.68531   38.92278   38.09674   37.23452
  0.08   35.90429   35.09863   37.62325   36.85956   36.04530   35.19866   39.31231   38.61070   37.83192   37.00829
  0.09   35.62882   34.86886   37.28343   36.57307   35.80265   34.99317   38.90459   38.26634   37.53808   36.75632
  0.10   35.32818   34.61665   36.91532   36.26051   35.53662   34.76703   38.46657   37.89270   37.21734   36.48011

  0.11   35.00448   34.34340   36.52211   35.92410   35.24876   34.52133   38.00270   37.49290   36.87191   36.18129
  0.12   34.65989   34.05059   36.10698   35.56611   34.94073   34.25725   37.51728   37.07007   36.50411   35.86157
  0.13   34.29663   33.73978   35.67311   35.18888   34.61420   33.97599   37.01442   36.62737   36.11629   35.52272
  0.14   33.91693   33.41255   35.22357   34.79474   34.27092   33.67883   36.49798   36.16786   35.71083   35.16654
  0.15   33.52301   33.07054   34.76133   34.38601   33.91266   33.36709   35.97154   35.69455   35.29009   34.79488

  0.16   33.11705   32.71540   34.28921   33.96498   33.54117   33.04209   35.43834   35.21028   34.85640   34.40958
  0.17   32.70117   32.34877   33.80983   33.53384   33.15823   32.70519   34.90131   34.71776   34.41201   34.01246
  0.18   32.27742   31.97228   33.32565   33.09474   32.76555   32.35775   34.36307   34.21951   33.95912   33.60532
  0.19   31.84775   31.58755   32.83890   32.64967   32.36483   32.00111   33.82591   33.71787   33.49979   33.18991
  0.20   31.41400   31.19614   32.35161   32.20056   31.95770   31.63660   33.29182   33.21498   33.03601   32.76793

  0.22   30.54104   30.39927   31.38256   31.29719   31.13041   30.88920   32.23955   32.21297   32.10231   31.91068
  0.24   29.67082   29.59298   30.43074   30.39724   30.29530   30.12552   31.21718   31.22663   31.17116   31.04557
  0.25   29.24001   29.18950   29.96432   29.95190   29.87805   29.74049   30.71970   30.74261   30.71004   30.61342
  0.26   28.81354   28.78733   29.50548   29.51116   29.46254   29.35476   30.23233   30.26609   30.25348   30.18314
  0.28   27.97732   27.99095   28.61349   28.64722   28.64081   28.58517   29.28998   29.33882   29.35803   29.33236
  0.30   27.16826   27.21097   27.75927   27.81166   27.83716   27.82387   28.39308   28.44996   28.49148   28.50055

  0.32   26.39067   26.45296   26.94549   27.00889   27.05714   27.07687   27.54293   27.60269   27.65860   27.69344
  0.34   25.64723   25.72106   26.17331   26.24170   26.30480   26.34897   26.73963   26.79860   26.86254   26.91530
  0.35   25.28876   25.36581   25.80284   25.87193   25.93991   25.99338   26.35530   26.41288   26.47889   26.53805
  0.36   24.93921   25.01803   25.44268   25.51149   25.58286   25.64386   25.98229   26.03799   26.10499   26.16902
  0.38   24.26676   24.34542   24.75264   24.81853   24.89288   24.96412   25.26931   25.32015   25.38646   25.45630
  0.40   23.62908   23.70373   24.10148   24.16216   24.23539   24.31138   24.59853   24.64360   24.70653   24.77783

  0.42   23.02466   23.09260   23.48700   23.54100   23.61007   23.68640   23.96741   24.00629   24.06398   24.13340
  0.44   22.45147   22.51097   22.90664   22.95314   23.01594   23.08919   23.37312   23.40576   23.45707   23.52215
  0.45   22.17586   22.23075   22.62838   22.67101   22.73011   22.80083   23.08887   23.11844   23.16630   23.22854
  0.46   21.90716   21.95728   22.35760   22.39633   22.45150   22.51915   22.81272   22.83929   22.88361   22.94266
  0.48   21.38915   21.42960   21.83701   21.86806   21.91488   21.97521   22.28316   22.30403   22.34116   22.39312
  0.50   20.89483   20.92579   21.34200   21.36572   21.40398   21.45594   21.78144   21.79707   21.82713   21.87145

  0.55   19.74591   19.75596   20.19825   20.20633   20.22447   20.25428   20.63000   20.63492   20.64909   20.67434
  0.60   18.69261   18.68755   19.15781   19.15478   19.15702   19.16707   19.59299   19.59062   19.59268   19.60165
  0.65   17.70659   17.69240   18.18958   18.17982   18.17126   18.16648   18.63663   18.62997   18.62393   18.62089
  0.70   16.76874   16.75034   17.27164   17.25866   17.24396   17.22966   17.73592   17.72728   17.71663   17.70590
  0.80   15.00071   14.98305   15.53914   15.52635   15.50916   15.48843   16.04176   16.03343   16.02079   16.00465
  0.90   13.36708   13.35491   13.92212   13.91318   13.89981   13.88201   14.45181   14.44614   14.43624   14.42216
  1.00   11.88982   11.88297   12.43544   12.43044   12.42201   12.40975   12.96965   12.96670   12.96051   12.95075

  1.10   10.59450   10.59126   11.10632   11.10410   11.09955   11.09217   11.62061   11.61958   11.61640   11.61058
  1.20    9.49290    9.49159    9.95334    9.95267    9.95051    9.94642   10.42764   10.42767   10.42639   10.42332
  1.30    8.58013    8.57961    8.98001    8.97997    8.97901    8.97678    9.40150    9.40194    9.40160    9.40011
  1.40    7.83843    7.83810    8.17620    8.17627    8.17576    8.17443    8.53952    8.53998    8.53997    8.53921
  1.50    7.24276    7.24237    7.52258    7.52253    7.52211    7.52116    7.82856    7.82885    7.82884    7.82833

  1.60    6.76558    6.76515    6.99520    6.99501    6.99456    6.99378    7.24906    7.24916    7.24903    7.24857
  1.70    6.38040    6.38000    6.56927    6.56899    6.56856    6.56793    6.77880    6.77874    6.77851    6.77806
  1.80    6.06373    6.06350    6.22160    6.22135    6.22102    6.22060    6.39567    6.39552    6.39526    6.39487
  1.90    5.79606    5.79610    5.93203    5.93189    5.93176    5.93164    6.07944    6.07929    6.07909    6.07884
  2.00    5.56198    5.56236    5.68392    5.68397    5.68412    5.68438    5.81276    5.81267    5.81260    5.81257

  2.50    4.59228    4.59430    4.71283    4.71408    4.71582    4.71804    4.82675    4.82737    4.82841    4.82988
  3.00    3.70819    3.71065    3.85042    3.85215    3.85449    3.85742    3.98636    3.98740    3.98904    3.99127
  3.50    2.93467    2.93668    3.07561    3.07713    3.07917    3.08169    3.21524    3.21622    3.21776    3.21982
  4.00    2.33507    2.33641    2.45577    2.45684    2.45828    2.46004    2.57925    2.57998    2.58112    2.58264
  5.00    1.61971    1.62011    1.69001    1.69036    1.69084    1.69141    1.76507    1.76534    1.76576    1.76631
  6.00    1.29098    1.29102    1.33058    1.33064    1.33072    1.33082    1.37295    1.37301    1.37309    1.37321
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Atom     Mo(5+)     Mo(6+)     Tc(1+)     Tc(2+)     Tc(3+)     Tc(4+)     Tc(5+)     Tc(6+)     Tc(7+)     Ru(1+)
   Z         42         42         43         43         43         43         43         43         43         44
Method      DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
  STL
  0.00   37.00000   36.00000   42.00000   41.00000   40.00000   39.00000   38.00000   37.00000   36.00000   43.00000
  0.01   36.98642   35.98850   41.96804   40.97714   39.98073   38.98356   37.98590   36.98790   35.98963   42.97279
  0.02   36.94574   35.95404   41.87282   40.90878   39.92309   38.93437   37.94369   36.95165   35.95858   42.89147
  0.03   36.87820   35.89679   41.71623   40.79559   39.82752   38.85272   37.87360   36.89142   35.90695   42.75704
  0.04   36.78416   35.81700   41.50131   40.63868   39.69476   38.73916   37.77601   36.80750   35.83497   42.57109
  0.05   36.66413   35.71504   41.23207   40.43955   39.52585   38.59442   37.65145   36.70028   35.74290   42.33578

  0.06   36.51877   35.59135   40.91328   40.20008   39.32205   38.41941   37.50060   36.57024   35.63113   42.05379
  0.07   36.34883   35.44650   40.55020   39.92245   39.08490   38.21523   37.32426   36.41800   35.50008   41.72821
  0.08   36.15522   35.28111   40.14840   39.60914   38.81613   37.98314   37.12337   36.24423   35.35027   41.36247
  0.09   35.93895   35.09591   39.71348   39.26286   38.51765   37.72453   36.89896   36.04973   35.18228   40.96024
  0.10   35.70111   34.89170   39.25091   38.88647   38.19153   37.44096   36.65219   35.83534   34.99673   40.52534

  0.11   35.44289   34.66934   38.76585   38.48294   37.83997   37.13404   36.38429   35.60200   34.79434   40.06170
  0.12   35.16556   34.42975   38.26307   38.05533   37.46523   36.80551   36.09658   35.35072   34.57585   39.57321
  0.13   34.87044   34.17392   37.74686   37.60670   37.06965   36.45715   35.79043   35.08254   34.34206   39.06369
  0.14   34.55890   33.90288   37.22103   37.14007   36.65560   36.09081   35.46726   34.79856   34.09382   38.53685
  0.15   34.23237   33.61769   36.68886   36.65841   36.22544   35.70836   35.12855   34.49994   33.83199   37.99621

  0.16   33.89225   33.31945   36.15318   36.16457   35.78150   35.31165   34.77578   34.18782   33.55748   37.44508
  0.17   33.54001   33.00927   35.61640   35.66128   35.32606   34.90255   34.41044   33.86342   33.27122   36.88653
  0.18   33.17708   32.68827   35.08051   35.15110   34.86133   34.48291   34.03404   33.52791   32.97416   36.32339
  0.19   32.80488   32.35761   34.54721   34.63643   34.38943   34.05450   33.64805   33.18251   32.66724   35.75824
  0.20   32.42483   32.01840   34.01790   34.11949   33.91237   33.61908   33.25393   32.82840   32.35144   35.19338

  0.22   31.64659   31.31880   32.97575   33.08672   32.95025   32.73378   32.44695   32.09880   31.69700   34.07254
  0.24   30.85280   30.59820   31.96134   32.06677   31.98860   31.83940   31.62391   31.34826   31.01840   32.97454
  0.25   30.45308   30.23263   31.46622   31.56515   31.51163   31.39229   31.20950   30.96785   30.67234   32.43743
  0.26   30.05297   29.86485   30.97985   31.07065   31.03891   30.94689   30.79470   30.58540   30.32295   31.90963
  0.28   29.25558   29.12633   30.03499   30.10671   30.11051   30.06560   29.96811   29.81814   29.61754   30.88511
  0.30   28.46793   28.38950   29.12936   29.18089   29.21066   29.20325   29.15175   29.05357   28.90852   29.90588

  0.32   27.69611   27.66031   28.26466   28.29709   28.34467   28.36598   28.35197   28.29787   28.20164   28.97485
  0.34   26.94501   26.94386   27.44182   27.45751   27.51619   27.55840   27.57388   27.55628   27.50195   28.09337
  0.35   26.57842   26.59174   27.04618   27.05459   27.11674   27.16679   27.19425   27.19214   27.15618   27.67129
  0.36   26.21833   26.24429   26.66102   26.66293   26.72736   26.78372   26.82142   26.83306   26.81378   27.26156
  0.38   25.51871   25.56485   25.92184   25.91308   25.97909   26.04396   26.09741   26.13156   26.14072   26.47856
  0.40   24.84780   24.90794   25.22326   25.20677   25.27127   25.34004   25.40366   25.45425   25.48566   25.74280

  0.42   24.20638   24.27514   24.56379   24.54220   24.60296   24.67201   24.74111   24.80278   24.85075   25.05214
  0.44   23.59450   23.66734   23.94156   23.91709   23.97260   24.03918   24.10992   24.17805   24.23752   24.40406
  0.45   23.29949   23.37291   23.64374   23.61852   23.67104   23.73558   23.80596   23.87584   23.93935   24.09513
  0.46   23.01160   23.08478   23.35439   23.32883   23.37818   23.44027   23.50962   23.58037   23.64690   23.79578
  0.48   22.45661   22.52720   22.79987   22.77463   22.81734   22.87357   22.93923   23.00946   23.07928   23.22435
  0.50   21.92811   21.99388   22.27547   22.25160   22.28755   22.33707   22.39736   22.46463   22.53461   22.68673

  0.55   20.71124   20.75916   21.07923   21.06140   21.08145   21.11309   21.15605   21.20896   21.26957   21.47095
  0.60   19.61938   19.64693   20.01562   20.00498   20.01212   20.02740   20.05204   20.08639   20.13000   20.40286
  0.65   18.62307   18.63230   19.04956   19.04535   19.04322   19.04562   19.05435   19.07077   19.09562   19.44317
  0.70   17.69709   17.69218   18.15274   18.15339   18.14540   18.13881   18.13548   18.13710   18.14504   18.56011
  0.80   15.98607   15.96630   16.49019   16.49570   16.48358   16.46896   16.45300   16.43698   16.42231   16.93558
  0.90   14.40411   14.38247   14.93773   14.94350   14.93293   14.91858   14.90081   14.88018   14.85743   15.41951
  1.00   12.93715   12.91957   13.47789   13.48191   13.47466   13.46381   13.44925   13.43098   13.40913   13.98150

  1.10   11.60171   11.58942   12.12734   12.12932   12.12517   12.11817   12.10798   12.09432   12.07700   12.63238
  1.20   10.41804   10.41015   10.90973   10.91017   10.90819   10.90417   10.89772   10.88847   10.87608   11.39585
  1.30    9.39710    9.39222    9.84152    9.84107    9.84035    9.83824    9.83438    9.82843    9.82004   10.29227
  1.40    8.53743    8.53437    8.92740    8.92663    8.92648    8.92539    8.92308    8.91929    8.91371    9.33200
  1.50    7.82716    7.82511    8.16111    8.16039    8.16037    8.15973    8.15826    8.15576    8.15199    8.51454

  1.60    7.24766    7.24619    7.52847    7.52797    7.52789    7.52740    7.52635    7.52459    7.52197    7.83066
  1.70    6.77732    6.77624    7.01085    7.01061    7.01043    7.00997    7.00914    7.00785    7.00599    7.26541
  1.80    6.39432    6.39358    6.58809    6.58808    6.58784    6.58741    6.58676    6.58583    6.58455    6.80098
  1.90    6.07854    6.07817    6.24065    6.24079    6.24056    6.24023    6.23978    6.23920    6.23843    6.41902
  2.00    5.81259    5.81265    5.95090    5.95112    5.95097    5.95080    5.95062    5.95042    5.95017    6.10217

  2.50    4.83177    4.83408    4.93622    4.93602    4.93688    4.93809    4.93966    4.94159    4.94390    5.04027
  3.00    3.99404    3.99734    4.11770    4.11704    4.11859    4.12067    4.12326    4.12637    4.12998    4.23841
  3.50    3.22235    3.22536    3.35468    3.35400    3.35555    3.35760    3.36013    3.36312    3.36658    3.48705
  4.00    2.58450    2.58669    2.70624    2.70577    2.70697    2.70855    2.71050    2.71278    2.71541    2.83137
  5.00    1.76698    1.76777    1.84534    1.84526    1.84574    1.84637    1.84713    1.84803    1.84905    1.92916
  6.00    1.37334    1.37350    1.41843    1.41846    1.41858    1.41873    1.41892    1.41913    1.41937    1.46706
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Atom Z Method STL	Ru(2+) 44 DHF	Ru(3+) 44 DHF	Ru(4+) 44 DHF	Ru(5+) 44 DHF	Ru(6+) 44 DHF	Ru(7+) 44 DHF	Ru(8+) 44 DHF	Rh(1+) 45 DHF	Rh(2+) 45 DHF	Rh(3+) 45 DHF
0.00	42.00000	41.00000	40.00000	39.00000	38.00000	37.00000	36.00000	44.00000	43.00000	42.00000
0.01	41.97731	40.98065	39.98332	38.98554	37.98745	36.98911	35.99059	43.97342	42.97756	41.98067
0.02	41.90946	40.92276	39.93338	38.94224	37.94985	36.95650	35.96241	43.89398	42.91044	41.92284
0.03	41.79706	40.82676	39.85050	38.87034	37.88738	36.90230	35.91555	43.76254	42.79920	41.82689
0.04	41.64113	40.69334	39.73520	38.77022	37.80033	36.82673	35.85017	43.58053	42.64479	41.69351
0.05	41.44306	40.52350	39.58818	38.64241	37.68912	36.73009	35.76651	43.34989	42.44849	41.52361
0.06	41.20460	40.31845	39.41036	38.48760	37.55424	36.61278	35.66487	43.07302	42.21191	41.31836
0.07	40.92780	40.07966	39.20280	38.30660	37.39633	36.47527	35.54559	42.75271	41.93696	41.07915
0.08	40.61496	39.80878	38.96675	38.10034	37.21609	36.31810	35.40910	42.39207	41.62579	40.80754
0.09	40.26863	39.50767	38.70359	37.86988	37.01434	36.14189	35.25585	41.99447	41.28076	40.50531
0.10	39.89151	39.17831	38.41483	37.61638	36.79197	35.94734	35.08638	41.56345	40.90444	40.17437
0.11	39.48644	38.82284	38.10209	37.34109	36.54995	35.73518	34.90125	41.10264	40.49950	39.81674
0.12	39.05634	38.44346	37.76707	37.04533	36.28930	35.50622	34.70108	40.61572	40.06870	39.43456
0.13	38.60415	38.04246	37.41156	36.73050	36.01113	35.26131	34.48653	40.10631	39.61487	39.03004
0.14	38.13282	37.62215	37.03738	36.39804	35.71657	35.00135	34.25829	39.57798	39.14083	38.60542
0.15	37.64523	37.18486	36.64639	36.04944	35.40681	34.72727	34.01708	39.03414	38.64939	38.16297
0.16	37.14421	36.73290	36.24048	35.68622	35.08306	34.44003	33.76367	38.47806	38.14329	37.70496
0.17	36.63246	36.26853	35.82150	35.30989	34.74655	34.14062	33.49883	37.91280	37.62521	37.23361
0.18	36.11256	35.79397	35.39130	34.92198	34.39853	33.83004	33.22336	37.34122	37.09769	36.75113
0.19	35.58694	35.31135	34.95170	34.52400	34.04023	33.50931	32.93805	36.76593	36.56318	36.25963
0.20	35.05787	34.82271	34.50445	34.11745	33.67290	33.17943	32.64375	36.18934	36.02395	35.76116
0.22	33.99756	33.83497	33.59377	33.28439	32.91603	32.49630	32.03141	35.04069	34.93975	34.75098
0.24	32.94631	32.84479	32.67195	32.43392	32.13742	31.78863	31.39291	33.90997	33.86025	33.73490
0.25	32.42789	32.35262	32.21045	32.00538	31.74279	31.42800	31.06587	33.35500	33.32629	33.22861
0.26	31.91596	31.86417	31.75029	31.57624	31.34603	31.06408	30.73468	32.80853	32.79800	32.72535
0.28	30.91572	30.90303	30.83857	30.72049	30.55008	30.32989	30.06290	31.74481	31.76301	31.73276
0.30	29.95239	29.96924	29.94495	29.87461	29.75696	29.59269	29.38338	30.72477	30.76290	30.76560
0.32	29.03068	29.06875	29.07603	29.04528	28.97313	28.85848	28.70152	29.75226	29.80320	29.83048
0.34	28.15349	28.20579	28.23685	28.23797	28.20408	28.13251	28.02218	28.82944	28.88760	28.93223
0.35	27.73209	27.78928	27.82962	27.84395	27.82654	27.77406	27.68483	28.38696	28.44704	28.49802
0.36	27.32225	27.38306	27.43109	27.45693	27.45430	27.41930	27.34967	27.95711	28.01820	28.07416
0.38	26.53719	26.60196	26.66115	26.70527	26.72736	26.72258	26.68772	27.13500	27.19584	27.25824
0.40	25.79757	25.86280	25.92831	25.98508	26.02590	26.04533	26.03944	26.36196	26.42032	26.48526
0.42	25.10192	25.16500	25.23294	25.29754	25.35174	25.38983	25.40739	25.63625	25.69057	25.75510
0.44	24.44822	24.50730	24.57461	24.64303	24.70594	24.75766	24.79351	24.95562	25.00494	25.06684
0.45	24.13636	24.19294	24.25903	24.32808	24.39382	24.45066	24.49386	24.63140	24.67801	24.73797
0.46	23.83406	23.88790	23.95226	24.02124	24.08890	24.14981	24.19925	24.31747	24.36127	24.41898
0.48	23.25675	23.30460	23.36436	23.43135	23.50046	23.56670	23.62552	23.71901	23.75707	23.80956
0.50	22.71347	22.75496	22.80900	22.87207	22.93996	23.00829	23.07280	23.15729	23.18965	23.23630
0.55	21.48516	21.51094	21.54845	21.59667	21.65361	21.71662	21.78266	21.89409	21.91333	21.94470
0.60	20.40748	20.41975	20.44105	20.47198	20.51230	20.56102	20.61657	20.79624	20.80492	20.82238
0.65	19.44118	19.44317	19.45094	19.46589	19.48891	19.52024	19.55959	19.82254	19.82352	19.82963
0.70	18.55408	18.54904	18.54676	18.54886	18.55672	18.57137	18.59338	18.93842	18.93432	18.93256
0.80	16.92695	16.91574	16.90303	16.89003	16.87803	16.86835	16.86223	17.33778	17.32947	17.31952
0.90	15.41222	15.40126	15.38700	15.36997	15.35084	15.33045	15.30974	15.85946	15.85162	15.84054
1.00	13.97674	13.96856	13.95687	13.94169	13.92317	13.90157	13.87732	14.45359	14.44798	14.43901
1.10	12.62993	12.62481	12.61671	12.60538	12.59064	12.57240	12.55065	13.11978	13.11655	13.11050
1.20	11.39502	11.39230	11.38732	11.37972	11.36921	11.35551	11.33840	11.87815	11.87675	11.87325
1.30	10.29234	10.29116	10.28836	10.28360	10.27657	10.26694	10.25442	10.75082	10.75057	10.74885
1.40	9.33243	9.33205	9.33056	9.32766	9.32307	9.31650	9.30767	9.75282	9.75314	9.75247
1.50	8.51500	8.51493	8.51410	8.51228	8.50925	8.50478	8.49861	8.88931	8.88979	8.88961
1.60	7.83099	7.83095	7.83039	7.82915	7.82706	7.82395	7.81962	8.15633	8.15675	8.15672
1.70	7.26556	7.26544	7.26497	7.26404	7.26252	7.26031	7.25725	7.54318	7.54344	7.54339
1.80	6.80097	6.80078	6.80034	6.79960	6.79849	6.79692	6.79479	7.03508	7.03518	7.03504
1.90	6.41891	6.41868	6.41831	6.41775	6.41698	6.41594	6.41456	6.61550	6.61546	6.61527
2.00	6.10204	6.10185	6.10159	6.10126	6.10083	6.10029	6.09958	6.26789	6.26779	6.26759
2.50	5.04065	5.04132	5.04229	5.04356	5.04514	5.04705	5.04928	5.14301	5.14329	5.14380
3.00	4.23934	4.24077	4.24270	4.24510	4.24798	4.25134	4.25519	4.35371	4.35456	4.35587
3.50	3.48807	3.48961	3.49164	3.49413	3.49709	3.50051	3.50438	3.61669	3.61770	3.61922
4.00	2.83221	2.83346	2.83510	2.83711	2.83947	2.84218	2.84525	2.95752	2.95840	2.95969
5.00	1.92952	1.93007	1.93077	1.93163	1.93263	1.93378	1.93507	2.01739	2.01781	2.01842
6.00	1.46717	1.46732	1.46752	1.46775	1.46802	1.46834	1.46868	1.51915	1.51928	1.51947

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Atom     Rh(4+)      Rh(5+)      Rh(6+)      Pd(2+)      Pd(4+)      Ag(1+)      Ag(2+)      Ag(3+)      Cd(2+)      In(1+)
   Z         45          45          45          46          46          47          47          47          48          49
Method      DHF         DHF         DHF         DHF         DHF         DHF         DHF         DHF         DHF         DHF
  STL
  0.00   41.00000    40.00000    39.00000    44.00000    42.00000    46.00000    45.00000    44.00000    46.00000    48.00000
  0.01   40.98318    39.98529    38.98711    43.97786    41.98313    45.97467    44.97819    43.98091    45.97854    47.96958
  0.02   40.93284    39.94125    38.94851    43.91162    41.93263    45.89892    44.91292    43.92376    45.91430    47.87880
  0.03   40.84927    39.86810    38.88437    43.80180    41.84877    45.77344    44.80467    43.82890    45.80773    47.72904
  0.04   40.73297    39.76623    38.79499    43.64926    41.73205    45.59938    44.65425    43.69694    45.65956    47.52254
  0.05   40.58464    39.63616    38.68078    43.45520    41.58312    45.37832    44.46273    43.52867    45.47080    47.26231

  0.06   40.40514    39.47857    38.54225    43.22109    41.40281    45.11221    44.23151    43.32514    45.24273    46.95196
  0.07   40.19552    39.29425    38.38003    42.94871    41.19213    44.80334    43.96220    43.08756    44.97684    46.59561
  0.08   39.95698    39.08413    38.19485    42.64005    40.95223    44.45430    43.65667    42.81734    44.67488    46.19771
  0.09   39.69086    38.84927    37.98751    42.29733    40.68440    44.06791    43.31698    42.51607    44.33875    45.76287
  0.10   39.39863    38.59079    37.75893    41.92294    40.39006    43.64718    42.94536    42.18546    43.97053    45.29576

  0.11   39.08187    38.30995    37.51008    41.51939    40.07073    43.19525    42.54418    41.82735    43.57246    44.80094
  0.12   38.74225    38.00806    37.24201    41.08930    39.72804    42.71533    42.11590    41.44369    43.14684    44.28280
  0.13   38.38151    37.68651    36.95583    40.63535    39.36367    42.21066    41.66306    41.03649    42.69608    43.74542
  0.14   38.00145    37.34674    36.65269    40.16025    38.97937    41.68446    41.18823    40.60784    42.22262    43.19260
  0.15   37.60390    36.99024    36.33379    39.66670    38.57694    41.13988    40.69401    40.15985    41.72893    42.62774

  0.16   37.19072    36.61851    36.00037    39.15735    38.15819    40.57998    40.18296    39.69464    41.21747    42.05390
  0.17   36.76376    36.23309    35.65367    38.63481    37.72494    40.00772    39.65759    39.21434    40.69067    41.47373
  0.18   36.32485    35.83551    35.29497    38.10159    37.27900    39.42587    39.12036    38.72106    40.15091    40.88959
  0.19   35.87581    35.42729    34.92553    37.56010    36.82218    38.83709    38.57364    38.21684    39.60052    40.30347
  0.20   35.41841    35.00994    34.54663    37.01263    36.35623    38.24381    38.01970    37.70369    39.04170    39.71710

  0.22   34.48532    34.15371    33.76540    35.90821    35.40375    37.05270    36.89861    36.65826    37.90724    38.54926
  0.24   33.53845    33.27812    32.96103    34.80383    34.43452    35.86851    35.77275    35.59923    36.76320    37.39539
  0.25   33.06354    32.83638    32.55307    34.25584    33.94736    35.28319    35.21233    35.06871    36.19196    36.82591
  0.26   32.58942    32.39364    32.14273    33.71257    33.46035    34.70426    34.65559    34.53952    35.62331    36.26235
  0.28   31.64836    31.50970    31.31902    32.64510    32.49169    33.57028    33.55836    33.49037    34.49923    35.15532
  0.30   30.72388    30.63457    30.49758    31.60983    31.53754    32.47441    32.49013    32.46123    33.40058    34.07834

  0.32   29.82303    29.77532    29.68514    30.61307    30.60538    31.42234    31.45791    31.45984    32.33500    33.03466
  0.34   28.95136    28.93776    28.88751    29.65926    29.70126    30.41795    30.46690    30.49226    31.30836    32.02695
  0.35   28.52782    28.52861    28.49578    29.19940    29.26122    29.93440    29.98802    30.02262    30.81103    31.53726
  0.36   28.11302    28.12653    28.10946    28.75124    28.82982    29.46353    29.52065    29.56301    30.32491    31.05733
  0.38   27.31087    27.34510    27.35485    27.89051    27.99440    28.56013    28.62131    28.67521    29.38744    30.12745
  0.40   26.54663    26.59591    26.62657    27.07742    27.19721    27.70777    27.76987    27.83080    28.49756    29.23849

  0.42   25.82105    25.88045    25.92669    26.31144    26.43942    26.90563    26.96630    27.03062    27.65582    28.39113
  0.44   25.13404    25.19938    25.25649    25.59129    25.72134    26.15225    26.20983    26.27467    26.86192    27.58561
  0.45   24.80479    24.87176    24.93273    25.24786    25.37708    25.79325    25.84883    25.91307    26.48264    27.19848
  0.46   24.48484    24.55266    24.61656    24.91517    25.04254    25.44568    25.49903    25.56221    26.11490    26.82170
  0.48   23.87213    23.93966    24.00690    24.28086    24.40201    24.78359    24.83201    24.89191    25.41321    26.09878
  0.50   23.29418    23.35925    23.42700    23.68584    23.79825    24.16340    24.20650    24.26200    24.75491    25.41586

  0.55   21.98763    22.04042    22.10061    22.35232    22.43701    22.77796    22.80762    22.84959    23.28371    23.87438
  0.60   20.84946    20.88618    20.93178    21.20385    21.25918    21.59261    21.61027    21.63818    22.02943    22.54740
  0.65   19.84294    19.86385    19.89297    20.15987    20.22784    20.56434    20.57239    20.58790    20.95059    21.40274
  0.70   18.93473    18.94221    18.95608    19.29964    19.30819    19.65471    19.65570    19.66133    20.00807    20.40682
  0.80   17.30907    17.29933    17.29154    17.70652    17.69031    18.06871    18.06210    18.05572    18.40065    18.73691
  0.90   15.82674    15.81084    15.79362    16.26223    16.23831    16.65393    16.64563    16.63518    17.00426    17.33017
  1.00   14.42673    14.41127    14.39289    14.89360    14.87139    15.31974    15.31270    15.30268    15.70538    16.05341

  1.10   13.10141    13.08913    13.07357    13.58524    13.56836    14.03787    14.03303    14.02531    14.45794    14.83985
  1.20   11.86730    11.85862    11.84698    12.35041    12.33921    12.81444    12.81171    12.80657    13.25714    13.66910
  1.30   10.74531    10.73963    10.73152    11.21066    11.20402    11.66899    11.66785    11.66486    12.11778    12.54700
  1.40    9.75049     9.74693     9.74151    10.18427    10.18070    10.62138    10.62124    10.61975    11.05961    11.49007
  1.50    8.88853     8.88629     8.88268     9.28131     9.27955     9.68540     9.68575     9.68516    10.09910    10.51551

  1.60    8.15605     8.15458     8.15211     8.50306     8.50218     8.86667     8.86718     8.86703     9.24593     9.63604
  1.70    7.54289     7.54183     7.54007     7.84336     7.84280     8.16328     8.16375     8.16375     8.50245     8.85795
  1.80    7.03461     7.03378     7.03249     7.29094     7.29043     7.56749     7.56781     7.56780     7.86472     8.18128
  1.90    6.61487     6.61423     6.61329     6.83161     6.83108     7.06775     7.06791     7.06784     7.32427     7.60097
  2.00    6.26727     6.26683     6.26621     6.45022     6.44970     6.65061     6.65064     6.65050     6.86981     7.10841

  2.50    5.14454     5.14553     5.14679     5.24609     5.24699     5.35114     5.35124     5.35147     5.46090     5.57670
  3.00    4.35763     4.35983     4.36248     4.46325     4.46601     4.56550     4.56617     4.56721     4.66433     4.76019
  3.50    3.62120     3.62365     3.62654     3.74235     3.74575     3.86067     3.86164     3.86305     3.97538     4.08634
  4.00    2.96138     2.96343     2.96585     3.08350     3.08653     3.20579     3.20672     3.20806     3.32738     3.44787
  5.00    2.01920     2.02015     2.02126     2.10974     2.11127     2.20435     2.20487     2.20560     2.30272     2.40445
  6.00    1.51971     1.52000     1.52034     1.57489     1.57541     1.63385     1.63405     1.63432     1.69674     1.76341
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Atom    In(2+)     In(3+)     Sn(2+)     Sn(4+)     Sb(3+)     Sb(5+)     Te(2+)     Te(4+)     Te(5+)     Te(6+)
   Z       49         49         50         50         51         51         52         52         52         52
Method    DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
  0.00  47.00000   46.00000   48.00000   46.00000   48.00000   46.00000   50.00000   48.00000   47.00000   46.00000
  0.01  46.97615   45.98130   47.97435   45.98341   47.97770   45.98511   49.97007   47.98026   46.98357   45.98652
  0.02  46.90485   45.92529   47.89769   45.93373   47.91101   45.94051   49.88067   47.92117   46.93437   45.94611
  0.03  46.78680   45.83229   47.77086   45.85119   47.80049   45.86637   49.73302   47.82317   46.85266   45.87892
  0.04  46.62314   45.70281   47.59526   45.73616   47.64713   45.76299   49.52910   47.68696   46.73889   45.78519
  0.05  46.41546   45.53757   47.37278   45.58919   47.45221   45.63079   49.27156   47.51350   46.59366   45.66524

  0.06  46.16568   45.33747   47.10573   45.41095   47.21739   45.47028   48.96369   47.30401   46.41774   45.51950
  0.07  45.87607   45.10360   46.79683   45.20226   46.94457   45.28211   48.60924   47.05991   46.21204   45.34847
  0.08  45.54912   44.83718   46.44906   44.96405   46.63592   45.06700   48.21239   46.78285   45.97761   45.15273
  0.09  45.18756   44.53963   46.06565   44.69738   46.29380   44.82580   47.77756   46.47461   45.71562   44.93296
  0.10  44.79422   44.21247   45.64997   44.40343   45.92074   44.55941   47.30933   46.13715   45.42735   44.68989

  0.11  44.37204   43.85734   45.20544   44.08347   45.51935   44.26885   46.81229   45.77252   45.11417   44.42434
  0.12  43.92397   43.47601   44.73550   43.73885   45.09233   43.95520   46.29099   45.38286   44.77754   44.13719
  0.13  43.45291   43.07029   44.24351   43.37101   44.64238   43.61961   45.74977   44.97034   44.41896   43.82937
  0.14  42.96174   42.64207   43.73271   42.98144   44.17217   43.26328   45.19276   44.53717   44.03998   43.50187
  0.15  42.45321   42.19331   43.20620   42.57170   43.68434   42.88746   44.62380   44.08556   43.64218   43.15571

  0.16  41.92995   41.72596   42.66686   42.14336   43.18141   42.49346   44.04634   43.61765   43.22716   42.79199
  0.17  41.39444   41.24201   42.11738   41.69806   42.66581   42.08261   43.46352   43.13558   42.79650   42.41180
  0.18  40.84901   40.74342   41.56021   41.23741   42.13984   41.65626   42.87804   42.64138   42.35180   42.01627
  0.19  40.29582   40.23214   40.99756   40.76304   41.60563   41.21578   42.29228   42.13701   41.89460   41.60657
  0.20  39.73688   39.71010   40.43143   40.27659   41.06516   40.76254   41.70821   41.62432   41.42644   41.18386

  0.22  38.60895   38.64113   39.29559   39.27385   39.97262   39.82331   40.55142   40.58087   40.46306   40.30412
  0.24  37.47808   37.55075   38.16443   38.24166   38.87490   38.84941   39.41729   39.52360   39.47289   39.38646
  0.25  36.91497   37.00164   37.60350   37.71825   38.32738   38.35277   38.86060   38.99319   38.97099   38.91630
  0.26  36.35496   36.45196   37.04691   37.19185   37.78224   37.85135   38.31144   38.46318   38.46615   38.44012
  0.28  35.24834   35.35639   35.94977   36.13533   36.70274   36.83909   37.23666   37.40843   37.45203   37.47404
  0.30  34.16532   34.27417   34.87806   35.08198   35.64266   35.82186   36.19389   36.36649   36.43864   36.49671

  0.32  33.11164   33.21388   33.83559   34.04053   34.60677   34.80811   35.18300   35.34299   35.43302   35.51604
  0.34  32.09185   32.18255   32.82529   33.01849   33.59869   33.80537   34.20337   34.34235   34.44119   34.53929
  0.35  31.59580   31.67956   32.33291   32.51678   33.10596   33.31023   33.72507   33.85169   33.95207   34.05445
  0.36  31.10945   31.18580   31.84938   32.02221   32.62114   32.82023   33.25435   33.36793   33.46824   33.57297
  0.38  30.16704   30.22785   30.90957   31.05684   31.67616   31.85831   32.33540   32.42228   32.51839   32.62287
  0.40  29.26640   29.31173   30.00715   30.12643   30.76526   30.92428   31.44622   31.50730   31.59511   31.69396

  0.42  28.40860   28.43934   29.14299   29.23397   29.88950   30.02190   30.58677   30.62437   30.70113   30.79045
  0.44  27.59404   27.61166   28.31761   28.38153   29.04960   29.15405   29.75720   29.77444   29.83861   29.91576
  0.45  27.20295   27.21467   27.91953   27.97073   28.64324   28.73375   29.35369   29.36207   29.41965   29.49010
  0.46  26.82257   26.82884   27.53118   27.57032   28.24597   28.32281   28.95776   28.95815   29.00911   29.07261
  0.48  26.09353   26.09035   26.78354   26.80081   27.47872   27.52951   28.18879   28.17584   28.21372   28.26302
  0.50  25.40585   25.39511   26.07418   26.07283   26.74769   26.77484   27.45056   27.42757   27.45306   27.48838

  0.55  23.85752   23.83535   24.46253   24.42896   25.07531   25.05662   25.74032   25.70442   25.70409   25.70866
  0.60  22.52915   22.50389   23.06569   23.01781   23.61355   23.56862   24.22140   24.18484   24.16766   24.15071
  0.65  21.38644   21.36337   21.85779   21.80852   22.34262   22.28792   22.88494   22.85425   22.82869   22.80004
  0.70  20.39415   20.37597   20.80938   20.76662   21.23801   21.18512   21.71533   21.69299   21.66561   21.63345
  0.80  18.73225   18.72537   19.07330   19.05206   19.42125   19.38872   19.79274   19.78596   19.76606   19.74160
  0.90  17.33126   17.33258   17.64842   17.64608   17.96173   17.95219   18.27451   18.27698   18.26867   18.25804
  1.00  16.05721   16.06241   16.38646   16.39482   16.70191   16.70771   16.99996   17.00575   17.00643   17.00684

  1.10  14.84409   14.84992   15.20278   15.21453   15.54159   15.55399   15.85448   15.85998   15.86537   15.87165
  1.20  13.67255   13.67726   14.06230   14.07288   14.43179   14.44352   14.77198   14.77565   14.78221   14.79000
  1.30  12.54925   12.55226   12.96131   12.96872   13.35484   13.36463   13.72480   13.72638   13.73196   13.73861
  1.40  11.49119   11.49261   11.91179   11.91576   12.31941   12.32524   12.71015   12.71003   12.71374   12.71812
  1.50  10.51580   10.51604   10.93028   10.93145   11.33871   11.34095   11.73816   11.73693   11.73870   11.74072

  1.60   9.63583    9.63537   10.03133   10.03065   10.42783   10.42744   10.82312   10.82136   10.82156   10.82170
  1.70   8.85752    8.85678    9.22436    9.22274    9.59845    9.59654    9.97812    9.97627    9.97545    9.97434
  1.80   8.18084    8.18010    8.51292    8.51108    8.85718    8.85468    9.21232    9.21066    9.20933    9.20762
  1.90   7.60063    7.60008    7.89526    7.89367    8.20539    8.20298    8.53007    8.52877    8.52735    8.52552
  2.00   7.10823    7.10792    7.36551    7.36441    7.64005    7.63814    7.93124    7.93034    7.92909    7.92749

  2.50   5.57690    5.57720    5.70123    5.70190    5.83594    5.83669    5.98202    5.98229    5.98259    5.98294
  3.00   4.75995    4.75964    4.85302    4.85268    4.94482    4.94479    5.03727    5.03708    5.03723    5.03742
  3.50   4.08571    4.08485    4.19077    4.18914    4.29019    4.28854    4.38596    4.38503    4.38431    4.38348
  4.00   3.44717    3.44622    3.56376    3.56175    3.67585    3.67354    3.78517    3.78384    3.78267    3.78128
  5.00   2.40410    2.40362    2.50765    2.50652    2.61235    2.61087    2.71922    2.71799    2.71714    2.71612
  6.00   1.76334    1.76326    1.83356    1.83332    1.90717    1.90679    1.98481    1.98404    1.98378    1.98348
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Atom      I(1+)      I(3+)      I(5+)      I(7+)      I(1-)      Xe(2+)     Xe(4+)     Xe(6+)     Xe(8+)     Cs(1+)
   Z         53         53         53         53         53         54         54         54         54         55
Method      DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
  STL
 0.00     52.00000   50.00000   48.00000   46.00000   54.00000   52.00000   50.00000   48.00000   46.00000   54.00000
 0.01     51.96257   49.97409   47.98230   45.98770   53.94235   51.96813   49.97712   47.98398   45.98871   53.96229
 0.02     51.85092   49.89662   47.92930   45.95083   53.77122   51.87294   49.90868   47.93599   45.95488   53.84972
 0.03     51.66688   49.76843   47.84133   45.88951   53.49198   51.71564   49.79528   47.85629   45.89859   53.66389
 0.04     51.41349   49.59087   47.71892   45.80394   53.11301   51.49821   49.63790   47.74531   45.82001   53.40744
 0.05     51.09477   49.36578   47.56282   45.69437   52.64507   51.22334   49.43790   47.60362   45.71936   53.08392

 0.06     50.71566   49.09545   47.37395   45.56115   52.10045   50.89437   49.19697   47.43197   45.59691   52.69773
 0.07     50.28178   48.78254   47.15343   45.40468   51.49219   50.51515   48.91709   47.23122   45.45301   52.25393
 0.08     49.79927   48.43006   46.90252   45.22546   50.83331   50.09000   48.60052   47.00240   45.28805   51.75813
 0.09     49.27457   48.04127   46.62264   45.02402   50.13628   49.62355   48.24974   46.74664   45.10249   51.21633
 0.10     48.71421   47.61958   46.31533   44.80097   49.41252   49.12064   47.86741   46.46517   44.89683   50.63474

 0.11     48.12468   47.16855   45.98222   44.55698   48.67218   48.58621   47.45629   46.15933   44.67162   50.01965
 0.12     47.51221   46.69176   45.62504   44.29277   47.92396   48.02520   47.01926   45.83053   44.42747   49.37728
 0.13     46.88268   46.19276   45.24556   44.00911   47.17513   47.44245   46.55920   45.48023   44.16503   48.71366
 0.14     46.24151   45.67503   44.84562   43.70683   46.43156   46.84260   46.07901   45.10996   43.88497   48.03449
 0.15     45.59355   45.14190   44.42705   43.38678   45.69782   46.23002   45.58152   44.72126   43.58803   47.34510

 0.16     44.94310   44.59653   43.99168   43.04986   44.97735   45.60879   45.06948   44.31569   43.27497   46.65035
 0.17     44.29385   44.04187   43.54135   42.69701   44.27257   44.98261   44.54554   43.89482   42.94657   45.95461
 0.18     43.64887   43.48063   43.07784   42.32917   43.58510   44.35478   44.01220   43.46021   42.60364   45.26169
 0.19     43.01068   42.91527   42.60289   41.94734   42.91582   43.72823   43.47179   43.01338   42.24703   44.57488
 0.20     42.38124   42.34796   42.11818   41.55250   42.26508   43.10544   42.92647   42.55584   41.87759   43.89693

 0.22     41.15416   41.21500   41.12585   40.72786   41.01848   41.87922   41.82879   41.61439   41.10372   42.57610
 0.24     39.97467   40.09417   40.11274   39.86341   39.84106   40.68853   40.73264   40.64683   40.28909   41.31158
 0.25     39.40353   39.54115   39.60174   39.41879   39.27615   40.10895   40.18851   40.15643   39.86872   40.70252
 0.26     38.84472   38.99417   39.08937   38.96726   38.72580   39.54061   39.64845   39.66315   39.44084   40.10937
 0.28     37.76291   37.92064   38.06473   38.04739   37.66476   38.43855   38.58385   38.67219   38.56606   38.97056
 0.30     36.72597   36.87681   37.04642   37.11147   36.65025   37.38247   37.54406   37.68164   37.67164   37.89283

 0.32     35.72984   35.86417   36.04067   36.16681   35.67549   36.37047   36.53233   36.69801   36.76427   36.87166
 0.34     34.77044   34.88307   35.05252   35.22023   34.73492   35.39958   35.55041   35.72676   35.85027   35.90149
 0.35     34.30337   34.40426   34.56631   34.74821   34.27608   34.92850   35.07087   35.24721   35.39266   35.43368
 0.36     33.84419   33.93320   34.08593   34.27802   33.82430   34.46641   34.59896   34.77234   34.93558   34.97642
 0.38     32.94816   33.01395   33.14402   33.34587   32.94063   33.56759   33.67794   33.83833   34.02568   34.09085
 0.40     32.08023   32.12467   32.22915   32.42884   32.08200   32.70014   32.78690   32.92754   33.12554   33.23979

 0.42     31.23899   31.26476   31.34308   31.53133   31.24738   31.86158   31.92524   32.04215   32.23963   32.41902
 0.44     30.42366   30.43382   30.48711   30.65712   30.43644   31.05003   31.09229   31.18382   31.37185   31.62523
 0.45     30.02562   30.02912   30.07071   30.22976   30.03988   30.65394   30.68640   30.76519   30.94585   31.23763
 0.46     29.63397   29.63159   29.66213   29.80934   29.64933   30.26414   30.28749   30.35374   30.52559   30.85589
 0.48     28.86997   28.85795   28.86870   28.99048   28.88651   29.50309   29.51035   29.55276   29.70368   30.10927
 0.50     28.13194   28.11290   28.10714   28.20249   28.14861   28.76641   28.76054   28.78139   28.90843   29.38423

 0.55     26.40295   26.37545   26.34260   26.37530   26.41719   27.03085   27.00406   26.98397   27.04766   27.66309
 0.60     24.84327   24.81600   24.77301   24.75689   24.85342   25.44846   25.41425   25.37209   25.37961   26.07304
 0.65     23.45245   23.42980   23.38802   23.34096   23.45855   24.02074   23.98771   23.93877   23.90536   24.61822
 0.70     22.22318   22.20670   22.17222   22.11092   22.22597   22.74518   22.71783   22.67222   22.61487   23.30144
 0.80     20.19093   20.18571   20.17032   20.11495   20.18983   20.61417   20.60141   20.57517   20.51098   21.07002
 0.90     18.59944   18.60095   18.59991   18.56991   18.59724   18.94354   18.94191   18.93476   18.89289   19.30834
 1.00     17.29410   17.29812   17.30401   17.29814   17.29223   17.59393   17.59797   17.60221   17.58731   17.89915

 1.10     16.15129   16.15522   16.16251   16.17171   16.15020   16.44028   16.44575   16.45410   16.45883   16.72105
 1.20     15.09076   15.09345   15.09918   15.11424   15.09041   15.39223   15.39676   15.40459   15.41904   15.67631
 1.30     14.07155   14.07276   14.07593   14.09041   14.07171   14.39675   14.39942   14.40459   14.42082   14.70045
 1.40     13.08110   13.08107   13.08179   13.09241   13.08153   13.43098   13.43178   13.43387   13.44711   13.75970
 1.50     12.12377   12.12293   12.12182   12.12766   12.12429   12.49226   12.49160   12.49109   12.49939   12.84316

 1.60     11.21161   11.21035   11.20816   11.20972   11.21209   11.58889   11.58731   11.58502   11.58835   11.95406
 1.70     10.35793   10.35656   10.35394   10.35241   10.35831   10.73313   10.73113   10.72790   10.72725   11.10247
 1.80      9.57366    9.57241    9.56985    9.56650    9.57393    9.93674    9.93470    9.93123    9.92795   10.30005
 1.90      8.86572    8.86471    8.86250    8.85848    8.86587    9.20851    9.20669    9.20346    9.19888    9.55688
 2.00      8.23666    8.23593    8.23422    8.23036    8.23672    8.55337    8.55191    8.54921    8.54439    8.87992

 2.50      6.14096    6.14113    6.14137    6.14171    6.14090    6.31374    6.31386    6.31392    6.31370    6.50066
 3.00      5.13144    5.13138    5.13134    5.13206    5.13151    5.22889    5.22894    5.22909    5.23017    5.33119
 3.50      4.47747    4.47690    4.47591    4.47459    4.47765    4.56520    4.56456    4.56361    4.56260    4.65083
 4.00      3.89002    3.88914    3.88753    3.88482    3.89026    3.98983    3.98869    3.98688    3.98410    4.08600
 5.00      2.82652    2.82563    2.82401    2.82173    2.82677    2.93313    2.93188    2.92988    2.92718    3.03998
 6.00      2.06559    2.06500    2.06396    2.06317    2.06579    2.14886    2.14801    2.14667    2.14560    2.23534
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Atom	Ba(2+)	La(2+)	La(3+)	Ce(2+)	Ce(3+)	Ce(4+)	Pr(2+)	Pr(3+)	Pr(4+)	Nd(2+)
Z	56	57	57	58	58	58	59	59	59	60
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	54.00000	55.00000	54.00000	56.00000	55.00000	54.00000	57.00000	56.00000	55.00000	58.00000
0.01	53.96738	54.96471	53.97121	55.96818	54.97161	53.97424	56.96869	55.97203	54.97460	57.96922
0.02	53.86989	54.85935	53.88512	55.87304	54.88670	53.89717	56.87510	55.88838	54.89861	57.87720
0.03	53.70866	54.68538	53.74254	55.71560	54.74605	53.76942	56.72015	55.74975	54.77262	57.72481
0.04	53.48549	54.44519	53.54483	55.49751	54.55092	53.59202	56.50540	55.55737	54.59759	57.51351
0.05	53.20290	54.14199	53.29382	55.22100	54.30305	53.36639	56.23299	55.31287	54.37487	57.24532
0.06	52.86397	53.77972	52.99182	54.88889	54.00462	53.09430	55.90554	55.01830	54.10614	56.92273
0.07	52.47235	53.36289	52.64156	54.50446	53.65822	52.77787	55.52617	54.67613	53.79341	56.54867
0.08	52.03209	52.89648	52.24613	54.07143	53.26678	52.41951	55.09839	54.28911	53.43897	56.12648
0.09	51.54764	52.38575	51.80893	53.59384	52.83352	52.02191	54.62604	53.86032	53.04535	55.65980
0.10	51.02370	51.83614	51.33359	53.07598	52.36190	51.58796	54.11321	53.39305	52.61531	55.15251
0.11	50.46510	51.25311	50.82395	52.52233	51.85559	51.12072	53.56417	52.89080	52.15178	54.60869
0.12	49.87678	50.64206	50.28394	51.93744	51.31834	50.62339	52.98322	52.35716	51.65781	54.03251
0.13	49.26363	50.00820	49.71755	51.32588	50.75401	50.09927	52.37491	51.79581	51.13655	53.42818
0.14	48.63045	49.35650	49.12878	50.69216	50.16642	49.55166	51.74344	51.21046	50.59120	52.79990
0.15	47.98186	48.69163	48.52154	50.04066	49.55938	48.98390	51.09310	50.60477	50.02495	52.15176
0.16	47.32223	48.01788	47.89966	49.37557	48.93659	48.39927	50.42797	49.98233	49.44097	51.48775
0.17	46.65566	47.33918	47.26677	48.70086	48.30163	47.80095	49.75193	49.34663	48.84238	50.81164
0.18	45.98590	46.65906	46.62633	48.02021	47.65788	47.19205	49.06863	48.70098	48.23218	50.12700
0.19	45.31634	45.98066	45.98157	47.33702	47.00852	46.57549	48.38142	48.04853	47.61326	49.43718
0.20	44.65001	45.30672	45.33544	46.65435	46.35652	45.95407	47.69337	47.39220	46.98835	48.74521
0.22	43.33713	43.98130	44.04960	45.30121	45.05516	44.70676	46.32552	46.07849	45.73066	47.36565
0.24	42.06381	42.69748	42.78694	43.97866	43.77224	43.46834	44.98340	44.77853	44.47735	46.00698
0.25	41.44557	42.07434	42.16871	43.33304	43.14230	42.85719	44.32639	44.13844	43.85714	45.34006
0.26	40.84089	41.46485	41.56101	42.69947	42.52197	42.25350	43.68052	43.50697	43.24340	44.68329
0.28	39.67432	40.28872	40.38106	41.47176	41.31440	41.07340	42.42588	42.27458	42.04047	43.40437
0.30	38.56608	39.17096	39.25252	40.29973	40.15589	39.93584	41.22467	41.08852	40.87700	42.17624
0.32	37.51512	38.11082	38.17760	39.18445	39.04961	38.84558	40.07892	39.95280	39.75849	41.00182
0.34	36.51837	37.10566	37.15601	38.12465	37.99617	37.80481	38.98823	38.86890	38.68791	39.88154
0.35	36.03899	36.62252	36.66460	37.61471	37.48890	37.30307	38.46292	38.34626	38.17092	39.34134
0.36	35.57148	36.15162	36.18561	37.11747	36.99422	36.81360	37.95049	37.83624	37.66608	38.81404
0.38	34.66955	35.24417	35.26305	36.15904	36.04110	35.87045	36.96245	36.85281	36.69219	37.79669
0.40	33.80762	34.37856	34.38430	35.24506	35.13326	34.97275	36.02025	35.91564	35.76422	36.82611
0.42	32.98102	33.55015	33.54507	34.37115	34.26679	34.11717	35.11981	35.02120	34.87934	35.89856
0.44	32.18560	32.75464	32.74117	33.53315	33.43768	33.30005	34.25713	34.16575	34.03426	35.01027
0.45	31.79847	32.36803	32.35124	33.12642	33.03593	32.90476	33.83877	33.75150	33.62557	34.57970
0.46	31.41788	31.98826	31.96872	32.72731	32.64212	32.51770	33.42848	33.34564	33.22553	34.15761
0.48	30.67505	31.24779	31.22429	31.95037	31.87664	31.76656	32.63055	32.55743	32.44975	33.33729
0.50	29.95497	30.53064	30.50501	31.19963	31.13823	31.04340	31.86050	31.79804	31.70373	32.54640
0.55	28.24552	28.82782	28.80282	29.42446	29.39525	29.34050	30.04312	30.00948	29.95104	30.68285
0.60	26.65835	27.24123	27.22180	27.77966	27.78036	27.76407	28.36201	28.35638	28.33356	28.96186
0.65	25.19277	25.76611	25.75377	26.25726	26.28175	26.29773	26.80605	26.82378	26.83202	27.36956
0.70	23.85153	24.40417	24.39842	24.85598	24.89647	24.93595	25.37178	25.40621	25.43817	25.90038
0.80	21.54341	22.02834	22.03117	22.41662	22.46717	22.52670	22.86495	22.91255	22.96753	23.32416
0.90	19.69687	20.10091	20.10631	20.43857	20.48009	20.53362	20.82030	20.86188	20.91447	21.21166
1.00	18.22133	18.55589	18.56038	18.85421	18.88048	18.91736	19.17831	19.20625	19.24443	19.50975
1.10	17.00648	17.29647	17.29887	17.56829	17.58137	17.60208	17.85068	17.86561	17.88818	18.13661
1.20	15.95304	16.22537	16.22583	16.48431	16.48944	16.49950	16.74360	16.74983	16.76113	17.00158
1.30	14.98831	15.26443	15.26357	15.52266	15.52496	15.53055	15.77585	15.77820	15.78387	16.02278
1.40	14.06860	14.36145	14.35994	14.62785	14.63089	14.63664	14.88760	14.88976	14.89446	15.13692
1.50	13.17439	13.48854	13.48688	13.76774	13.77337	13.78183	14.04132	14.04544	14.05207	14.30171
1.60	12.30280	12.63624	12.63472	12.92884	12.93748	12.94941	13.21839	13.22527	13.23500	13.49366
1.70	11.46047	11.80692	11.80568	12.11024	12.12143	12.13641	12.41385	12.42332	12.43612	12.70368
1.80	10.65787	11.00898	11.00804	11.31820	11.33103	11.34801	11.63121	11.64258	11.65767	11.93225
1.90	9.90553	10.25260	10.25191	10.56185	10.57532	10.59307	10.87817	10.89054	10.90687	11.18527
2.00	9.21181	9.54697	9.54647	9.85030	9.86350	9.88088	10.16347	10.17599	10.19247	10.47071
2.50	6.70203	6.91767	6.91742	7.13311	7.13870	7.14616	7.36279	7.36897	7.37720	7.60026
3.00	5.43980	5.55618	5.55606	5.68130	5.68119	5.68110	5.81428	5.81462	5.81515	5.95578
3.50	4.73461	4.81773	4.81794	4.90456	4.90346	4.90198	4.99203	4.99098	4.98959	5.08233
4.00	4.17740	4.26438	4.26487	4.34953	4.34930	4.34889	4.43176	4.43139	4.43081	4.51224
5.00	3.14509	3.24795	3.24856	3.34751	3.34864	3.34997	3.44542	3.44645	3.44765	3.54085
6.00	2.32366	2.41346	2.41387	2.50328	2.50433	2.50561	2.59471	2.59577	2.59704	2.68677

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Atom    Nd(3+)    Pm(3+)    Sm(2+)    Sm(3+)    Eu(2+)    Eu(3+)    Gd(1+)    Gd(2+)    Gd(3+)    Tb(1+)
   Z       60        61        62        62        63        63        64        64        64        65
Method    DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF       DHF
  STL
  0.00  57.00000  58.00000  60.00000  59.00000  61.00000  60.00000  63.00000  62.00000  61.00000  64.00000
  0.01  56.97246  57.97289  59.97027  58.97332  60.97078  59.97374  62.95563  61.96869  60.97415  63.95847
  0.02  56.89008  57.89178  59.88135  58.89347  60.88336  59.89514  62.82373  61.87511  60.89677  63.83500
  0.03  56.75354  57.75733  59.73402  58.76109  60.73849  59.76479  62.60779  61.72029  60.76842  63.63292
  0.04  56.56397  57.57059  59.52960  58.57717  60.53742  59.58365  62.31333  61.50590  60.59002  63.35739
  0.05  56.32293  57.33305  59.26987  58.34311  60.28182  59.35305  61.94742  61.23422  60.36281  63.01498

  0.06  56.03237  57.04655  58.95706  58.06067  59.97382  59.07463  61.51815  60.90804  60.08838  62.61312
  0.07  55.69460  56.71328  58.59381  57.73192  59.61593  58.75039  61.03409  60.53060  59.76860  62.15955
  0.08  55.31226  56.33574  58.18311  57.35924  59.21097  58.38258  60.50375  60.10548  59.40563  61.66184
  0.09  54.88825  55.91670  57.72826  56.94527  58.76210  57.97371  59.93521  59.63653  59.00186  61.12701
  0.10  54.42573  55.45915  57.23277  56.49285  58.27265  57.52649  59.33578  59.12776  58.55988  60.56127

  0.11  53.92800  54.96627  56.70036  56.00500  57.74618  57.04382  58.71182  58.58326  58.08245  59.96996
  0.12  53.39853  54.44134  56.13485  55.48490  57.18635  56.52872  58.06872  58.00713  57.57247  59.35747
  0.13  52.84082  53.88776  55.54011  54.93577  56.59688  55.98429  57.41092  57.40342  57.03293  58.72741
  0.14  52.25846  53.30893  54.92003  54.36091  55.98150  55.41370  56.74199  56.77606  56.46685  58.08266
  0.15  51.65497  52.70829  54.27844  53.76360  55.34392  54.82013  56.06478  56.12884  55.87731  57.42561

  0.16  51.03383  52.08919  53.61907  53.14711  54.68776  54.20671  55.38158  55.46533  55.26734  56.75825
  0.17  50.39843  51.45491  52.94553  52.51463  54.01650  53.57655  54.69424  54.78892  54.63993  56.08232
  0.18  49.75202  50.80864  52.26123  51.86923  53.33350  52.93264  54.00432  54.10276  53.99802  55.39943
  0.19  49.09767  50.15337  51.56939  51.21387  52.64191  52.27787  53.31318  53.40975  53.34441  54.71111
  0.20  48.43828  49.49198  50.87301  50.55135  51.94469  51.61499  52.62205  52.71258  52.68180  54.01886

  0.22  47.11491  48.16123  49.47738  49.21518  50.54403  50.27508  51.24438  51.31522  51.33962  52.62856
  0.24  45.80068  46.83517  48.09332  47.87942  49.15051  48.93150  49.88004  49.92735  49.98988  51.24037
  0.25  45.15183  46.17881  47.41043  47.21666  48.46132  48.26332  49.20543  49.24120  49.31718  50.55061
  0.26  44.51061  45.52907  46.73570  46.55953  47.77930  47.59982  48.53714  48.56209  48.64820  49.86551
  0.28  43.25603  44.25472  45.41552  45.26765  46.44181  46.29245  47.22295  47.22936  47.32722  48.51398
  0.30  42.04478  43.02057  44.14024  44.01275  45.14610  45.01880  45.94360  45.93624  46.03670  47.19406

  0.32  40.88167  41.83211  42.91427  42.80092  43.89722  43.78550  44.70377  44.68734  44.78374  45.91203
  0.34  39.76894  40.69228  41.73956  41.63574  42.69777  42.59672  43.50664  43.48520  43.57310  44.67219
  0.35  39.23158  40.14094  41.17148  41.07120  42.11684  42.01975  42.92467  42.90201  42.98442  44.06892
  0.36  38.70675  39.60195  40.61610  40.51874  41.54839  41.45456  42.35392  42.33073  42.40722  43.47698
  0.38  37.69376  38.56040  39.54250  39.44979  40.44824  40.35946  41.24605  41.22349  41.28729  42.32731
  0.40  36.72753  37.56574  38.51637  38.42754  39.39544  39.31062  40.18241  40.16209  40.21291  41.22282

  0.42  35.80498  36.61534  37.53476  37.44982  38.38746  38.30628  39.16159  39.14448  39.18279  40.16228
  0.44  34.92270  35.70614  36.59445  36.51392  37.42139  37.34412  38.18161  38.16819  38.19497  39.14380
  0.45  34.49557  35.26597  36.13877  36.06074  36.95313  36.87804  37.70623  37.69470  37.71620  38.64964
  0.46  34.07721  34.83490  35.69220  35.61689  36.49421  36.42149  37.24018  37.23053  37.24710  38.16514
  0.48  33.26520  33.99846  34.82487  34.75574  35.60294  35.53559  36.33484  36.32881  36.33661  37.22388
  0.50  32.48359  33.19382  33.98961  33.92757  34.74480  34.68367  35.46315  35.46039  35.46093  36.31760

  0.55  30.64591  31.30445  32.02587  31.98472  32.72851  32.68615  33.41613  33.41956  33.40805  34.19007
  0.60  28.95111  29.56517  30.21721  30.19880  30.87321  30.85193  31.53415  31.54077  31.52433  32.23605
  0.65  27.38159  27.95624  28.54553  28.54837  29.15921  29.15829  29.79537  29.80277  29.78611  30.43342
  0.70  25.92955  26.46775  27.00150  27.02168  27.57560  27.59191  28.18639  28.19299  28.17873  28.76814
  0.80  23.36901  23.83784  24.28048  24.32004  24.77937  24.81634  25.33139  25.33446  25.32729  25.81945
  0.90  21.25318  21.65520  22.02808  22.06896  22.45497  22.49526  22.93643  22.93625  22.93477  23.34987
  1.00  19.53921  19.88070  20.19989  20.23186  20.56076  20.59369  20.96746  20.96552  20.96700  21.32007

  1.10  18.15337  18.44626  18.72546  18.74573  19.03113  19.05303  19.36932  19.36698  19.36927  19.67270
  1.20  17.00908  17.26908  17.52120  17.53156  17.78623  17.79811  18.07016  18.06824  18.07010  18.33561
  1.30  16.02547  16.26880  16.50606  16.51010  16.74616  16.75115  16.99382  16.99263  16.99356  17.23277
  1.40  15.13853  15.37914  15.61215  15.61347  15.84179  15.84332  16.07091  16.07042  16.07039  16.29439
  1.50  14.30463  14.55253  14.78947  14.79076  15.02011  15.02094  15.24547  15.24551  15.24468  15.46318

  1.60  13.49900  13.75974  14.00579  14.00866  14.24510  14.24703  14.47720  14.47754  14.47618  14.69677
  1.70  12.71156  12.98658  13.24391  13.24901  13.49574  13.49964  13.74059  13.74105  13.73938  13.96714
  1.80  11.94221  12.22972  12.49787  12.50515  12.76272  12.76876  13.02232  13.02276  13.02098  13.25845
  1.90  11.19654  11.49254  11.76902  11.77803  12.04488  12.05276  12.31808  12.31842  12.31665  12.56413
  2.00  10.48249  10.78179  11.06282  11.07292  11.34598  11.35515  11.62945  11.62965  11.62798  11.88394

  2.50   7.60698   7.85137   8.09326   8.10077   8.34606   8.35383   8.61036   8.61015   8.60921   8.85800
  3.00   5.95660   6.10720   6.26453   6.26632   6.43143   6.43371   6.60950   6.60941   6.60895   6.78859
  3.50   5.08137   5.17541   5.27447   5.27381   5.37762   5.37716   5.48598   5.48603   5.48593   5.60051
  4.00   4.51176   4.59107   4.67062   4.66998   4.74986   4.74917   4.82906   4.82909   4.82930   4.91165
  5.00   3.54179   3.63452   3.72384   3.72457   3.81132   3.81194   3.89625   3.89615   3.89665   3.97850
  6.00   2.68783   2.78019   2.87146   2.87251   2.96345   2.96448   3.05547   3.05535   3.05581   3.14536
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Atom	Tb(3+)	Tb(4+)	Dy(2+)	Dy(3+)	Ho(3+)	Er(3+)	Tm(2+)	Tm(3+)	Yb(2+)	Yb(3+)
Z	65	65	66	66	67	68	69	69	70	70
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	62.00000	61.00000	64.00000	63.00000	64.00000	65.00000	67.00000	66.00000	68.00000	67.00000
0.01	61.97455	60.97675	63.97221	62.97494	63.97532	64.97569	66.97352	65.97605	67.97392	66.97640
0.02	61.89836	60.90715	63.88906	62.89992	63.90144	64.90291	66.89425	65.90435	67.89587	66.90574
0.03	61.77198	60.79163	63.75119	62.77544	63.77882	64.78212	66.76276	65.78532	67.76638	66.78844
0.04	61.59625	60.63089	63.55965	62.60233	63.60827	64.61405	66.57996	65.61969	67.58631	66.62517
0.05	61.37237	60.42591	63.31590	62.38173	63.39085	64.39976	66.34710	65.40843	67.35687	66.41688
0.06	61.10186	60.17792	63.02174	62.11505	63.12794	64.14052	66.06576	65.15279	67.07957	66.16475
0.07	60.78649	59.88841	62.67935	61.80401	62.82116	63.83791	65.73782	64.85426	66.75620	65.87021
0.08	60.42831	59.55906	62.29116	61.45057	62.47237	63.49370	65.36542	64.51454	66.38882	65.53488
0.09	60.02961	59.19177	61.85991	61.05690	62.08366	63.10988	64.95094	64.13553	65.97970	65.16060
0.10	59.59287	58.78860	61.38851	60.62536	61.65729	62.68862	64.49695	63.71931	65.53132	64.74935
0.11	59.12072	58.35179	60.88007	60.15850	61.19569	62.23225	64.00619	63.26812	65.04630	64.30328
0.12	58.61594	57.88367	60.33781	59.65896	60.70141	61.74321	63.48152	62.78430	64.52739	63.82464
0.13	58.08140	57.38668	59.76503	59.12950	60.17709	61.22404	62.92588	62.27030	63.97743	63.31579
0.14	57.52001	56.86335	59.16508	58.57294	59.62543	60.67736	62.34226	61.72863	63.39931	62.77916
0.15	56.93473	56.31621	58.54128	57.99210	59.04919	60.10581	61.73366	61.16185	62.79592	62.21719
0.16	56.32850	55.74784	57.89692	57.38985	58.45110	59.51204	61.10307	60.57252	62.17016	61.63239
0.17	55.70422	55.16081	57.23520	56.76899	57.83390	58.89870	60.45342	59.96320	61.52488	61.02722
0.18	55.06473	54.55763	56.55922	56.13227	57.20026	58.26839	59.78757	59.33642	60.86285	60.40415
0.19	54.41277	53.94080	55.87194	55.48238	56.55279	57.62363	59.10827	58.69464	60.18677	59.76557
0.20	53.75099	53.31272	55.17617	54.82189	55.89400	56.96691	58.41816	58.04027	59.49921	59.11382
0.22	52.40780	52.03193	53.76945	53.47881	54.55200	55.62684	57.01535	56.70289	58.09931	57.77979
0.24	51.05338	50.73246	52.35779	52.12102	53.19199	54.26565	55.59723	55.34144	56.68103	56.41891
0.25	50.37694	50.08053	51.65508	51.44156	52.51015	53.58201	54.88738	54.65652	55.96991	55.73318
0.26	49.70332	49.42944	50.95671	50.76404	51.82941	52.89866	54.17930	53.97112	55.25976	55.04622
0.28	48.37043	48.13578	49.57855	49.42081	50.47726	51.53889	52.77428	52.60494	53.84829	53.67472
0.30	47.06479	46.86204	48.23264	48.10163	49.14605	50.19703	51.39229	51.25370	52.45691	52.31527
0.32	45.79387	45.61653	46.92558	46.81436	47.84393	48.88147	50.04098	49.92601	51.09352	50.97670
0.34	44.56285	44.40539	45.66161	45.56458	46.57685	47.59849	48.72580	48.62846	49.76391	49.66581
0.35	43.96335	43.81409	45.04656	44.95494	45.95778	46.97067	48.08294	47.99252	49.11306	49.02239
0.36	43.37487	43.23283	44.44301	44.35588	45.34884	46.35250	47.45032	47.36577	48.47201	48.38765
0.38	42.23142	42.10138	43.27051	43.19022	44.16225	45.14625	46.21655	46.14107	47.22018	47.14569
0.40	41.13263	41.01216	42.14362	42.06817	43.01810	43.98114	45.02524	44.95613	46.00955	45.94202
0.42	40.07765	39.96517	41.06103	40.98929	41.91633	42.85748	43.87615	43.81161	44.84022	44.77765
0.44	39.06488	38.95951	40.02081	39.95235	40.85606	41.77476	42.76837	42.70732	43.71158	43.65270
0.45	38.57369	38.47173	39.51590	39.44908	40.34105	41.24841	42.22954	42.17002	43.16218	43.10486
0.46	38.09227	37.99368	39.02073	38.95561	39.83585	40.73182	41.70048	41.64242	42.62248	42.56662
0.48	37.15750	37.06577	38.05840	37.99700	38.85391	39.72712	40.67074	40.61560	41.57141	41.51834
0.50	36.25818	36.17363	37.13141	37.07431	37.90821	38.75886	39.67727	39.62527	40.55668	40.50650
0.55	34.14969	34.08517	34.95384	34.91026	35.68895	36.48497	37.33973	37.29750	38.16715	38.12577
0.60	32.21561	32.17362	32.95233	32.92532	33.65290	34.39778	35.18892	35.15938	35.96690	35.93706
0.65	30.43175	30.41275	31.10457	31.09499	31.77554	32.47304	33.20223	33.18707	33.93361	33.91717
0.70	28.78231	28.78449	29.39608	29.40262	30.03956	30.69294	31.36329	31.36249	32.05066	32.04789
0.80	25.85327	25.88593	26.36511	26.39450	26.95112	27.52316	28.08831	28.11057	28.69320	28.71323
0.90	23.38801	23.43256	23.81775	23.85534	24.33705	24.83333	25.31052	25.34428	25.83761	25.86992
1.00	21.35253	21.39456	21.71619	21.75081	22.16229	22.58735	22.99159	23.02623	23.44480	23.47912
1.10	19.69543	19.72755	20.00627	20.03231	20.38061	20.74092	21.08484	21.11371	21.46986	21.49935
1.20	18.34883	18.36952	18.61896	18.63539	18.93075	19.23578	19.53074	19.55121	19.85603	19.87766
1.30	17.23887	17.25013	17.47996	17.48843	17.74347	18.00512	18.26203	18.27438	18.53849	18.55210
1.40	16.29633	16.30150	16.51942	16.52265	16.75074	16.98195	17.21145	17.21747	17.45130	17.45838
1.50	15.46358	15.46595	15.67847	15.67914	15.89283	16.10606	16.31816	16.32014	16.53364	16.53629
1.60	14.69750	14.69961	14.91211	14.91235	15.12210	15.32812	15.53167	15.53174	15.73390	15.73419
1.70	13.96929	13.97276	14.18926	14.19044	14.40401	14.61118	14.81337	14.81316	15.01151	15.01112
1.80	13.26244	13.26801	13.49103	13.49386	13.71608	13.93003	14.13610	14.13671	14.33701	14.33711
1.90	12.56990	12.57765	12.80815	12.81280	13.04582	13.26958	13.48278	13.48477	13.69086	13.69215
2.00	11.89116	11.90077	12.13830	12.14458	12.38831	12.62261	12.84431	12.84785	13.06176	13.06450
2.50	8.86565	8.87600	9.11397	9.12194	9.37698	9.62976	9.87201	9.87941	10.11805	10.12511
3.00	6.79160	6.79577	6.97741	6.98100	7.17649	7.37735	7.57824	7.58280	7.78724	7.79203
3.50	5.60054	5.60061	5.72095	5.72124	5.84818	5.98144	6.11982	6.12098	6.26520	6.26666
4.00	4.91102	4.91012	4.99555	4.99491	5.08152	5.17137	5.26526	5.26490	5.36270	5.36247
5.00	3.97886	3.97926	4.05840	4.05870	4.13636	4.21212	4.28626	4.28627	4.35917	4.35910
6.00	3.14626	3.14739	3.23465	3.23558	3.32356	3.41004	3.49411	3.49489	3.57729	3.57800

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Atom     Lu(3+)     Hf(2+)     Hf(3+)     Hf(4+)     Ta(2+)     Ta(3+)     Ta(4+)     Ta(5+)     W(1+)      W(2+)
    Z      71         72         72         72         73         73         73         73         74         74
Method    DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
  0.00   68.00000   70.00000   69.00000   68.00000   71.00000   70.00000   69.00000   68.00000   73.00000   72.00000
  0.01   67.97674   69.97051   68.97535   67.97895   70.96974   69.97436   68.97789   67.98076   72.96018   71.96928
  0.02   67.90710   69.88236   68.90158   67.91590   70.87926   69.89764   68.91168   67.92314   72.84145   71.87743
  0.03   67.79147   69.73645   68.77920   67.81117   70.72951   69.77042   68.80175   67.82737   72.64592   71.72538
  0.04   67.63050   69.53427   68.60905   67.66526   70.52202   69.59363   68.64872   67.69388   72.37701   71.51464
  0.05   67.42510   69.27782   68.39229   67.47889   70.25885   69.36857   68.45343   67.52323   72.03922   71.24726

  0.06   67.17640   68.96958   68.13037   67.25294   69.94257   69.09686   68.21697   67.31615   71.63795   70.92579
  0.07   66.88575   68.61239   67.82501   66.98849   69.57613   68.78040   67.94062   67.07351   71.17921   70.55319
  0.08   66.55474   68.20943   67.47814   66.68678   69.16282   68.42135   67.62585   66.79632   70.66937   70.13275
  0.09   66.18509   67.76407   67.09191   66.34922   68.70618   68.02209   67.27429   66.48573   70.11492   69.66803
  0.10   65.77873   67.27984   66.66863   65.97733   68.20990   67.58516   66.88774   66.14298   69.52224   69.16277

  0.11   65.33771   66.76032   66.21074   65.57277   67.67775   67.11323   66.46811   65.76945   68.89742   68.62082
  0.12   64.86421   66.20909   65.72075   65.13731   67.11351   66.60906   66.01742   65.36659   68.24612   68.04602
  0.13   64.36049   65.62968   65.20127   64.67279   66.52089   66.07545   65.53775   64.93595   67.57349   67.44223
  0.14   63.82888   65.02549   64.65489   64.18116   65.90351   65.51523   65.03126   64.47913   66.88410   66.81316
  0.15   63.27177   64.39979   64.08422   63.66438   65.26481   64.93118   64.50012   63.99782   66.18196   66.16240

  0.16   62.69157   63.75566   63.49185   63.12447   64.60807   64.32604   63.94654   63.49372   65.47049   65.49337
  0.17   62.09066   63.09600   62.88030   62.56347   63.93633   63.70248   63.37270   62.96856   64.75262   64.80927
  0.18   61.47143   62.42351   62.25201   61.98343   63.25244   63.06306   62.78077   62.42411   64.03077   64.11308
  0.19   60.83623   61.74069   61.60936   61.38637   62.55900   62.41022   62.17286   61.86213   63.30697   63.40753
  0.20   60.18734   61.04981   60.95461   60.77429   61.85838   61.74629   61.55104   61.28437   62.58290   62.69514

  0.22   58.85723   59.65212   59.61729   59.51286   60.44402   60.39373   60.27362   60.08842   61.13920   61.25866
  0.24   57.49766   58.24505   58.25580   58.21417   59.02414   59.02110   58.96350   58.84973   59.70807   59.81907
  0.25   56.81154   57.54183   57.57037   57.55522   58.31590   58.33153   58.30047   58.21838   58.99912   59.10203
  0.26   56.12349   56.84055   56.88389   56.89205   57.61047   57.64180   57.63421   57.58103   58.29538   58.38853
  0.28   54.74766   55.44825   55.51324   55.55898   56.21222   56.26697   56.29767   56.29404   56.90544   56.97635
  0.30   53.38111   54.07582   54.15357   54.22590   54.83643   54.90567   54.96409   54.99934   55.54158   55.58948

  0.32   52.03279   52.72921   52.81274   52.90214   53.48839   53.56509   53.64205   53.70626   54.20644   54.23295
  0.34   50.70975   51.41287   51.49691   51.59545   52.17194   52.25073   52.33853   52.42278   52.90211   52.91023
  0.35   50.05942   50.76710   50.84988   50.95049   51.52642   51.60470   51.69550   51.78680   52.26203   52.26229
  0.36   49.41729   50.13002   50.21074   50.31202   50.88971   50.96665   51.05907   51.15563   51.63022   51.62357
  0.38   48.15919   48.88279   48.95755   49.05663   49.64338   49.71570   49.80786   49.91025   50.39195   50.37422
  0.40   46.93786   47.67241   47.73952   47.83278   48.43381   48.49969   48.58793   48.69089   49.18802   49.16269

  0.42   45.75464   46.49933   46.55789   46.64283   47.26122   47.31959   47.40130   47.50074   48.01876   47.98887
  0.44   44.60994   45.36345   45.41310   45.48818   46.12533   46.17567   46.24916   46.34202   46.88410   46.85220
  0.45   44.05196   44.80927   44.85448   44.92430   45.57094   45.61722   45.68618   45.77492   46.32963   46.29753
  0.46   43.50347   44.26414   44.30498   44.36942   45.02544   45.06768   45.13195   45.21615   45.78365   45.75177
  0.48   42.43444   43.20048   43.23290   43.28653   43.96056   43.99494   44.04960   44.12381   44.71674   44.68643
  0.50   41.40168   42.17126   42.19589   42.23898   42.92951   42.95648   43.00156   43.06515   43.68249   43.65484

  0.55   38.96900   39.73988   39.74845   39.76834   40.49100   40.50227   40.52555   40.56285   41.23259   41.21411
  0.60   36.73021   37.49314   37.49082   37.49362   38.23383   38.23395   38.24037   38.25550   38.96149   38.95270
  0.65   34.66287   35.41057   35.40195   35.39388   36.13782   36.13105   36.12610   36.12510   36.85050   36.84975
  0.70   32.74881   33.47555   33.46416   33.45042   34.18634   34.17611   34.16464   34.15352   34.88324   34.88811
  0.80   29.33099   30.00261   29.99199   29.97699   30.67064   30.66006   30.64565   30.62792   31.33150   31.34078
  0.90   26.41022   27.01365   27.00701   26.99666   27.62536   27.61827   27.60754   27.59308   28.24008   28.24788
  1.00   23.94612   24.47368   24.47089   24.46579   25.01799   25.01471   25.00897   25.00046   25.57485   25.57908

  1.10   21.89815   22.34838   22.34818   22.34692   22.81965   22.81913   22.81736   22.81401   23.30999   23.31086
  1.20   20.21566   20.59330   20.59440   20.59527   20.99240   20.99347   20.99408   20.99408   21.41350   21.41212
  1.30   18.83908   19.15388   19.15531   19.15695   19.48784   19.48934   19.49096   19.49255   19.84296   19.84055
  1.40   17.70568   17.97048   17.97167   17.97321   18.25022   18.25160   18.25329   18.25522   18.54794   18.54541
  1.50   16.75568   16.98441   16.98511   16.98609   17.22303   17.22395   17.22519   17.22672   17.47494   17.47285

  1.60   15.93670   16.14277   16.14290   16.14316   16.35354   16.35392   16.35448   16.35525   16.57241   16.57099
  1.70   15.20626   15.40128   15.40091   15.40046   15.59631   15.59617   15.59604   15.59597   15.79444   15.79371
  1.80   14.53230   14.72548   14.72471   14.72367   14.91482   14.91425   14.91352   14.91267   15.10291   15.10278
  1.90   13.89256   14.09047   14.08942   14.08794   14.28168   14.28080   14.27960   14.27812   14.46825   14.46854
  2.00   13.27316   13.47981   13.47858   13.47681   13.67792   13.67684   13.67532   13.67338   13.86908   13.86963

  2.50   10.36622   10.61323   10.61209   10.61028   10.85426   10.85320   10.85152   10.84918   11.08940   11.08978
  3.00    8.00425    8.22708    8.22638    8.22522    8.45247    8.45181    8.45071    8.44914    8.68033    8.68027
  3.50    6.41828    6.57919    6.57881    6.57821    6.74655    6.74618    6.74558    6.74474    6.92059    6.92052
  4.00    5.46441    5.57138    5.57127    5.57110    5.68376    5.68363    5.68342    5.68314    5.80194    5.80196
  5.00    4.43097    4.50127    4.50154    4.50193    4.57142    4.57165    4.57198    4.57242    4.64159    4.64155
  6.00    3.65932    3.73851    3.73891    3.73946    3.81607    3.81645    3.81698    3.81764    3.89179    3.89160
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Atom      W(3+)      W(4+)      W(5+)      W(6+)      Re(1+)     Re(2+)     Re(3+)     Re(4+)     Re(5+)     Re(6+)
    Z        74         74         74         74         75         75         75         75         75         75
Method        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
  STL
 0.00   71.00000   70.00000   69.00000   68.00000   74.00000   73.00000   72.00000   71.00000   70.00000   69.00000
 0.01   70.97366   69.97708   68.97989   67.98229   73.96052   72.96904   71.97318   70.97646   69.97919   68.98154
 0.02   70.89486   69.90844   68.91965   67.92924   73.84275   72.87646   71.89292   70.90598   69.91686   68.92624
 0.03   70.76418   69.79451   68.81958   67.84105   73.64862   72.72315   71.75983   70.78899   69.81334   68.83432
 0.04   70.58262   69.63596   68.68015   67.71806   73.38127   72.51058   71.57491   70.62622   69.66914   68.70619
 0.05   70.35155   69.43374   68.50203   67.56074   73.04487   72.24076   71.33954   70.41865   69.48500   68.54237

 0.06   70.07264   69.18903   68.28607   67.36970   72.64443   71.91614   71.05543   70.16752   69.26183   68.34355
 0.07   69.74790   68.90324   68.03328   67.14564   72.18559   71.53964   70.72461   69.87432   69.00073   68.11055
 0.08   69.37960   68.57799   67.74481   66.88940   71.67437   71.11447   70.34939   69.54073   68.70297   67.84430
 0.09   68.97023   68.21505   67.42197   66.60195   71.11699   70.64417   69.93230   69.16865   68.36995   67.54589
 0.10   68.52246   67.81640   67.06621   66.28431   70.51962   70.13243   69.47606   68.76011   68.00325   67.21650

 0.11   68.03910   67.38410   66.67906   65.93764   69.88824   69.58309   68.98356   68.31730   67.60452   66.85738
 0.12   67.52304   66.92034   66.26217   65.56317   69.22851   69.00002   68.45774   67.84251   67.17554   66.46993
 0.13   66.97723   66.42738   65.81727   65.16218   68.54565   68.38709   67.90164   67.33810   66.71816   66.05557
 0.14   66.40462   65.90752   65.34614   64.73605   67.84439   67.74810   67.31830   66.80649   66.23429   65.61582
 0.15   65.80815   65.36311   64.85061   64.28620   67.12895   67.08671   66.71074   66.25013   65.72590   65.15222

 0.16   65.19069   64.79648   64.33256   63.81409   66.40303   66.40644   66.08191   65.67146   65.19498   64.66638
 0.17   64.55500   64.20994   63.79387   63.32121   65.66982   65.71061   65.43469   65.07289   64.64351   64.15992
 0.18   63.90379   63.60578   63.23642   62.80910   64.93207   65.00231   64.77185   64.45679   64.07348   63.63447
 0.19   63.23957   62.98621   62.66207   62.27929   64.19208   64.28442   64.09604   63.82549   63.48687   63.09169
 0.20   62.56477   62.35338   62.07268   61.73331   63.45180   63.55957   63.40974   63.18119   62.88560   62.53319

 0.22   61.19225   61.05611   60.85596   60.59898   61.97660   62.09835   62.01486   61.86210   61.64657   61.37552
 0.24   59.80233   59.72931   59.60008   59.41817   60.51642   60.63499   60.60392   60.51532   60.37069   60.17403
 0.25   59.10519   59.05915   58.96151   58.81397   59.79420   59.90667   59.89692   59.83598   59.72308   59.56061
 0.26   58.40860   58.38658   58.31787   58.20245   59.07814   59.18240   59.19095   59.15479   59.07107   58.94063
 0.28   57.02216   57.03971   57.02093   56.96273   57.66655   57.75040   57.78737   57.79247   57.75946   57.68633
 0.30   55.65189   55.69866   55.71954   55.70903   56.28503   56.34624   56.40223   56.43835   56.44609   56.42113

 0.32   54.30467   54.37162   54.42257   54.45041   54.93597   54.97502   55.04242   55.10055   55.13971   55.15392
 0.34   52.98564   53.06513   53.13755   53.19487   53.62107   53.64016   53.71300   53.78548   53.84762   53.89243
 0.35   52.33790   52.42124   52.50150   52.57046   52.97680   52.98705   53.06085   53.13804   53.20882   53.26593
 0.36   51.69848   51.78429   51.87065   51.94933   52.34146   52.34372   52.41751   52.49800   52.57570   52.64323
 0.38   50.44566   50.53285   50.62680   50.71961   51.09778   51.08673   51.15818   51.24162   51.32857   51.41176
 0.40   49.22864   49.31347   49.40979   49.51049   49.89028   49.86938   49.93623   50.01872   50.10968   50.20240

 0.42   48.04808   48.12781   48.22240   48.32576   48.71884   48.69129   48.75207   48.83071   48.92151   49.01858
 0.44   46.90400   46.97677   47.06650   47.16830   47.58303   47.55160   47.60547   47.67823   47.76563   47.86281
 0.45   46.34551   46.41433   46.50074   46.60047   47.02826   46.99581   47.04606   47.11534   47.20010   47.29602
 0.46   45.79594   45.86059   45.94323   46.04018   46.48212   46.44916   46.49574   46.56129   46.64292   46.73685
 0.48   44.72308   44.77903   44.85308   44.94275   45.41521   45.38255   45.42184   45.47942   45.55364   45.64177
 0.50   43.68431   43.73142   43.79603   43.87675   44.38120   44.35026   44.38248   44.43179   44.49757   44.57809

 0.55   41.22801   41.25438   41.29479   41.34982   41.93196   41.90903   41.92563   41.95501   41.99830   42.05570
 0.60   38.95513   38.96482   38.98388   39.01390   39.66035   39.64724   39.65197   39.66474   39.68738   39.72118
 0.65   36.84472   36.84622   36.84543   36.85905   37.54659   37.54239   37.53966   37.53966   37.54597   37.55966
 0.70   34.87898   34.86963   34.86162   34.85654   35.57355   35.57614   35.56810   35.56077   35.55568   35.55435
 0.80   31.33024   31.31641   31.29991   31.28145   31.99907   32.00820   31.99770   31.98449   31.96924   31.95274
 0.90   28.24029   28.22918   28.21454   28.19643   28.86834   28.87720   28.86909   28.85764   28.84290   28.82502
 1.00   25.57521   25.56877   25.55948   25.54711   26.14855   26.15413   26.14962   26.14246   26.13243   26.11933

 1.10   23.30991   23.30752   23.30338   23.29719   23.81849   23.82044   23.81898   23.81592   23.81094   23.80376
 1.20   21.41290   21.41315   21.41260   21.41099   21.85253   21.85178   21.85228   21.85207   21.85089   21.84848
 1.30   19.84204   19.84355   19.84491   19.84594   20.21474   20.21251   20.21393   20.21525   20.21628   20.21684
 1.40   18.54691   18.54870   18.55066   18.55272   18.85989   18.85723   18.85882   18.86063   18.86255   18.86446
 1.50   17.47398   17.47544   17.47718   17.47918   17.73789   17.73550   17.73681   17.73844   17.74034   17.74246

 1.60   16.57160   16.57244   16.57353   16.57487   16.79869   16.79693   16.79775   16.79884   16.80021   16.80184
 1.70   15.79379   15.79396   15.79425   15.79468   15.99628   15.99524   15.99553   15.99598   15.99660   15.99742
 1.80   15.10240   15.10195   15.10147   15.10098   15.29130   15.29092   15.29074   15.29057   15.29042   15.29034
 1.90   14.46783   14.46688   14.46574   14.46444   14.65221   14.65235   14.65180   14.65110   14.65028   14.64937
 2.00   13.86869   13.86738   13.86574   13.86380   14.05536   14.05586   14.05504   14.05394   14.05259   14.05101

 2.50   11.08877   11.08717   11.08496   11.08212   11.31862   11.31912   11.31814   11.31660   11.31449   11.31180
 3.00    8.67963    8.67856    8.67703    8.67501    8.90957    8.90955    8.90893    8.90788    8.90637    8.90438
 3.50    6.92015    6.91954    6.91869    6.91757    7.10080    7.10073    7.10036    7.09975    7.09887    7.09772
 4.00    5.80180    5.80156    5.80123    5.80081    5.92620    5.92622    5.92604    5.92577    5.92539    5.92492
 5.00    4.64175    4.64204    4.64241    4.64287    4.71217    4.71215    4.71231    4.71255    4.71287    4.71326
 6.00    3.89196    3.89247    3.89309    3.89384    3.96536    3.96516    3.96551    3.96599    3.96658    3.96730
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Atom     Re(7+)     Os(1+)     Os(2+)     Os(3+)     Os(4+)     Os(5+)     Os(6+)     Os(7+)     Os(8+)     Ir(1+)
    Z        75         76         76         76         76         76         76         76         76         77
Method      DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
  0.00    68.00000   75.00000   74.00000   73.00000   72.00000   71.00000   70.00000   69.00000   68.00000   76.00000
  0.01    67.98361   74.96095   73.96895   72.97286   71.97600   70.97864   69.98092   68.98294   67.98475   75.96142
  0.02    67.93449   74.84439   73.87608   72.89162   71.90413   70.91465   69.92377   68.93183   67.93906   75.84624
  0.03    67.85282   74.65211   73.72226   72.75691   71.78485   70.80838   69.82879   68.84685   67.86307   75.65611
  0.04    67.73887   74.38699   73.50889   72.56969   71.61888   70.66038   69.69642   68.72834   67.75702   75.39367
  0.05    67.59305   74.05290   73.23788   72.33135   71.40723   70.47141   69.52723   68.57672   67.62124   75.06250

  0.06    67.41585   73.65447   72.91162   72.04359   71.15117   70.24243   69.32195   68.39257   67.45617   74.66692
  0.07    67.20788   73.19699   72.53290   71.70841   70.85222   69.97460   69.08148   68.17656   67.26230   74.21185
  0.08    66.96984   72.68613   72.10487   71.32813   70.51209   69.66923   68.80683   67.92947   67.04025   73.70264
  0.09    66.70253   72.12780   71.63094   70.90527   70.13273   69.32783   68.49916   67.65221   66.79068   73.14489
  0.10    66.40684   71.52794   71.11475   70.44257   69.71622   68.95200   68.15974   67.34575   66.51436   72.54427

  0.11    66.08373   70.89236   70.56006   69.94289   69.26480   68.54352   67.78994   67.01117   66.21212   71.90640
  0.12    65.73424   70.22663   69.97072   69.40924   68.78082   68.10422   67.39122   66.64962   65.88484   71.23673
  0.13    65.35949   69.53598   69.35057   68.84465   68.26670   67.63606   66.96514   66.26232   65.53348   70.54040
  0.14    64.96063   68.82521   68.70343   68.25222   67.72494   67.14102   66.51329   65.85055   65.15905   69.82224
  0.15    64.53889   68.09866   68.03299   67.63500   67.15804   66.62117   66.03735   65.41564   64.76260   69.08665

  0.16    64.09554   67.36021   67.34283   66.99602   66.56852   66.07857   65.53900   64.95897   64.34523   68.33763
  0.17    63.63187   66.61329   66.63634   66.33822   65.95886   65.51530   65.01996   64.48195   63.90808   67.57876
  0.18    63.14920   65.86087   65.91672   65.66444   65.33152   64.93344   64.48197   63.98600   63.45229   66.81320
  0.19    62.64888   65.10552   65.18695   64.97739   64.68888   64.33503   63.92676   63.47257   62.97906   66.04372
  0.20    62.13227   64.34942   64.44978   64.27966   64.03323   63.72208   63.35604   62.94309   62.48958   65.27272

  0.22    61.05559   62.84215   62.96307   62.86162   62.69166   62.46029   62.17482   61.84178   61.46670   63.73418
  0.24    59.92995   61.35066   61.47393   61.42767   61.32311   61.16287   60.95139   60.69340   60.39331   62.21078
  0.25    59.35206   60.61349   60.73288   60.70941   60.63330   60.50507   60.32773   60.10500   59.84065   61.45784
  0.26    58.76584   59.88310   59.99613   59.99244   59.94197   59.84331   59.69804   59.50889   59.27891   60.71199
  0.28    57.57331   58.44508   58.54024   58.56787   58.56054   58.51363   58.42604   58.29854   58.13271   59.24446
  0.30    56.36175   57.04040   57.11408   57.16337   57.18909   57.18424   57.14554   57.07189   56.96346   57.81271

  0.32    55.13982   55.67163   55.72312   55.78614   55.83588   55.86397   55.86543   55.83761   55.77934   56.41970
  0.34    53.91533   54.34036   54.37097   54.44139   54.50740   54.56009   54.59339   54.60341   54.58787   55.06723
  0.35    53.30433   53.68909   53.71016   53.78237   53.85401   53.91617   53.96244   53.98849   53.99153   54.40650
  0.36    52.69522   53.04748   53.05975   53.13269   53.20850   53.27842   53.33583   53.37604   53.39583   53.75620
  0.38    51.48547   51.79334   51.79040   51.86226   51.94262   52.02342   52.09801   52.16123   52.20926   52.48682
  0.40    50.29118   50.57781   50.56299   50.63119   50.71200   50.79840   50.88409   50.96381   51.03339   51.25879

  0.42    49.11655   49.40041   49.37692   49.43975   49.51790   49.60562   49.69722   49.78767   49.87268   50.07137
  0.44    47.96495   48.26036   48.23112   48.28751   48.36078   48.44644   48.53968   48.63586   48.73084   48.92349
  0.45    47.39863   47.70402   47.67289   47.72583   47.79604   47.87969   47.97240   48.06982   48.16796   48.36399
  0.46    46.83898   47.15662   47.12417   47.17359   47.24044   47.32153   47.41295   47.51068   47.61088   47.81387
  0.48    45.74054   46.08799   46.05443   46.09672   46.15624   46.23094   46.31789   46.41374   46.51512   46.74101
  0.50    44.67090   45.05312   45.02013   45.05541   45.10714   45.17427   45.25479   45.34608   45.44531   45.70332

  0.55    42.12664   42.60413   42.57741   42.59687   42.62929   42.67539   42.73504   42.80736   42.89100   43.25185
  0.60    39.76683   40.33410   40.31678   40.32390   40.33970   40.36574   40.40301   40.45191   40.51236   40.98334
  0.65    37.58203   38.22129   38.21336   38.21182   38.21501   38.22464   38.24214   38.26862   38.30482   38.87343
  0.70    35.55820   36.24711   36.24689   36.24000   36.23466   36.23236   36.23454   36.24251   36.25740   36.90144
  0.80    31.93586   32.66008   32.66850   32.65810   32.64553   32.63156   32.61701   32.60280   32.58991   33.31076
  0.90    28.80422   29.49970   29.50928   29.50067   29.48891   29.47416   29.45662   29.43661   29.41453   30.13028
  1.00    26.10300   26.73318   26.74001   26.73484   26.72697   26.71623   26.70249   26.68565   26.66570   27.32547

  1.10    23.79412   24.34326   24.34638   24.34437   24.34058   24.33475   24.32661   24.31592   24.30246   24.88203
  1.20    21.84459   22.31056   22.31059   22.31074   22.31002   22.30814   22.30484   22.29994   22.29312   22.78634
  1.30    20.21674   20.60572   20.60385   20.60514   20.60620   20.60682   20.60681   20.60598   20.60413   21.01569
  1.40    18.86626   19.18925   19.18659   19.18822   19.18999   19.19178   19.19346   19.19490   19.19599   19.53661
  1.50    17.74474   18.01502   18.01241   18.01386   18.01562   18.01761   18.01976   18.02202   18.02432   18.30753

  1.60    16.80373   17.03513   17.03303   17.03405   17.03537   17.03697   17.03883   17.04093   17.04325   17.28329
  1.70    15.99844   16.20403   16.20265   16.20315   16.20386   16.20479   16.20594   16.20733   16.20896   16.41939
  1.80    15.29036   15.48156   15.48090   15.48091   15.48100   15.48118   15.48148   15.48193   15.48254   15.67538
  1.90    14.64842   14.83455   14.83449   14.83411   14.83364   14.83314   14.83261   14.83210   14.83164   15.01680
  2.00    14.04923   14.23730   14.23767   14.23699   14.23610   14.23502   14.23379   14.23243   14.23097   14.41611

  2.50    11.30851   11.54113   11.54176   11.54079   11.53931   11.53729   11.53472   11.53160   11.52792   11.75660
  3.00     8.90188    9.13934    9.13939    9.13876    9.13772    9.13623    9.13425    9.13177    9.12877    9.36876
  3.50     7.09628    7.28681    7.28673    7.28636    7.28574    7.28485    7.28367    7.28218    7.28038    7.47812
  4.00     5.92433    6.05668    6.05669    6.05650    6.05620    6.05578    6.05525    6.05458    6.05379    6.19348
  5.00     4.71373    4.78367    4.78366    4.78379    4.78399    4.78425    4.78458    4.78497    4.78542    4.85658
  6.00     3.96813    4.03704    4.03684    4.03718    4.03763    4.03820    4.03888    4.03967    4.04057    4.10701
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Atom	Ir(2+)	Ir(3+)	Ir(4+)	Ir(5+)	Ir(6+)	Pt(2+)	Pt(4+)	Pt(5+)	Pt(6+)	Au(1+)
Z	77	77	77	77	77	78	78	78	78	79
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	75.00000	74.00000	73.00000	72.00000	71.00000	76.00000	74.00000	73.00000	72.00000	78.00000
0.01	74.96897	73.97265	72.97566	71.97820	70.98042	75.96907	73.97542	72.97786	71.98001	77.96503
0.02	74.87614	73.89082	72.90277	71.91292	70.92175	75.87652	73.90181	72.91157	71.92012	77.86047
0.03	74.72235	73.75507	72.78180	71.80449	70.82428	75.72314	73.77963	72.80147	71.82062	77.68735
0.04	74.50891	73.56640	72.61346	71.65348	70.68843	75.51019	73.60958	72.64812	71.68194	77.44735
0.05	74.23766	73.32612	72.39876	71.46068	70.51481	75.23941	73.39268	72.45232	71.50472	77.14276
0.06	73.91087	73.03591	72.13898	71.22706	70.30421	74.91296	73.13017	72.21505	71.28975	76.77642
0.07	73.53124	72.69776	71.83564	70.95382	70.05754	74.53340	72.82357	71.93751	71.03797	76.35167
0.08	73.10177	72.31392	71.49047	70.64230	69.77588	74.10363	72.47459	71.62106	70.75050	75.87222
0.09	72.62578	71.88690	71.10541	70.29403	69.46043	73.62681	72.08516	71.26725	70.42857	75.34212
0.10	72.10678	71.41938	70.68256	69.91068	69.11253	73.10636	71.65738	70.87776	70.07354	74.76563
0.11	71.54845	70.91423	70.22419	69.49406	68.73360	72.54582	71.19350	70.45441	69.68689	74.14717
0.12	70.95457	70.37441	69.73266	69.04605	68.32519	71.94827	70.69587	69.99913	69.27019	73.49122
0.13	70.32892	69.80298	69.21043	68.56866	67.88891	71.31924	70.16697	69.51393	68.82511	72.80225
0.14	69.67529	69.20301	68.66003	68.06394	67.42644	70.66063	69.60932	69.00090	68.35337	72.08465
0.15	68.99737	68.57759	68.08399	67.53400	66.93951	69.97672	69.02547	68.46219	67.85676	71.34268
0.16	68.29876	67.92976	67.48487	66.98097	66.42989	69.27110	68.41802	67.89996	67.33710	70.58043
0.17	67.58290	67.26251	66.86522	66.40699	65.89938	68.54720	67.78951	67.31639	66.79622	69.80175
0.18	66.85305	66.57872	66.22754	65.81420	65.34977	67.80833	67.14248	66.71365	66.23600	69.01029
0.19	66.11226	65.88116	65.57425	65.20470	64.78288	67.05761	66.47941	66.09391	65.65828	68.20940
0.20	65.36340	65.17248	64.90772	64.58055	64.20048	66.29796	65.80270	65.45927	65.06489	67.40217
0.22	63.85168	63.73154	63.54391	63.29634	62.99615	64.76246	64.41751	64.15348	63.83835	65.77968
0.24	62.33614	62.27388	62.15291	61.97680	61.75034	63.22091	63.00414	62.81193	62.57034	64.16209
0.25	61.58167	61.54364	61.45193	61.30818	61.11589	62.45287	62.29177	62.13227	61.92490	63.36003
0.26	60.83149	60.81473	60.74956	60.63584	60.47574	61.68890	61.57793	61.44892	61.27392	62.56458
0.28	59.34916	59.36666	59.34664	59.28582	59.18394	60.17874	60.15210	60.07722	59.96104	60.99865
0.30	57.89767	57.93963	57.95477	57.93747	57.88532	58.69977	58.73775	58.70788	58.64237	59.47264
0.32	56.48308	56.54125	56.58256	56.59982	56.58896	57.25874	57.34389	57.35028	57.32725	57.99228
0.34	55.10940	55.17711	55.23672	55.28030	55.30260	55.86021	55.97761	56.01209	56.02360	56.56112
0.35	54.43870	54.50912	54.57532	54.62924	54.66523	55.17782	55.30653	55.35224	55.37820	55.86464
0.36	53.77900	53.85098	53.92227	53.98481	54.03268	54.50697	54.64420	54.69942	54.73802	55.18104
0.38	52.49293	52.56522	52.64273	52.71784	52.78443	53.20034	53.34740	53.41693	53.47580	53.85258
0.40	51.25127	51.32096	51.40036	51.48265	51.56189	51.94055	52.08962	52.16795	52.24104	52.57525
0.42	50.05333	50.11841	50.19638	50.28144	50.36812	50.72696	50.87215	50.95472	51.03675	51.34782
0.44	48.89790	48.95708	49.03115	49.11546	49.20522	49.55830	49.69535	49.77848	49.86502	50.16854
0.45	48.33564	48.39156	48.46299	48.54587	48.63579	48.99031	49.12213	49.20440	49.29178	49.59628
0.46	47.78338	47.83591	47.90436	47.98523	48.07452	48.43288	48.55889	48.63970	48.72709	49.03524
0.48	46.70791	46.75348	46.81520	46.89065	46.97669	47.34869	47.46185	47.53819	47.62350	47.94554
0.50	45.66950	45.70811	45.76248	45.83115	45.91184	46.30356	46.40292	46.47326	46.55425	46.89692
0.55	43.22210	43.24465	43.28023	43.32918	43.39103	43.84672	43.91146	43.96333	44.02740	44.43831
0.60	40.96211	40.97177	40.99065	41.02002	41.06060	41.58509	41.61954	41.65227	41.69608	42.18170
0.65	38.86167	38.86202	38.86784	38.88069	38.90182	39.48753	39.49846	39.51453	39.53918	40.09267
0.70	36.89807	36.89241	36.88908	36.88951	36.89506	37.52848	37.52292	37.52609	37.53492	38.14300
0.80	33.31796	33.30771	33.29585	33.28319	33.27060	33.95355	33.93245	33.92116	33.91055	34.58135
0.90	30.14019	30.13111	30.11912	30.10443	30.08734	30.76632	30.74463	30.73009	30.71354	31.39162
1.00	27.33341	27.32756	27.31900	27.30761	27.29332	27.93092	27.91517	27.90319	27.88845	28.53382
1.10	24.88636	24.88374	24.87921	24.87251	24.86344	25.43772	25.42916	25.42162	25.41164	25.99966
1.20	22.78730	22.78704	22.78573	22.78311	22.77894	23.28023	23.27757	23.27418	23.26909	23.78753
1.30	21.01433	21.01543	21.01616	21.01630	21.01565	21.44328	21.44447	21.44406	21.44272	21.88870
1.40	19.53409	19.53571	19.53738	19.53897	19.54033	19.89994	19.90302	19.90433	19.90529	20.28261
1.50	18.30478	18.30635	18.30819	18.31020	18.31232	18.61353	18.61705	18.61903	18.62103	18.93788
1.60	17.28090	17.28211	17.28362	17.28540	17.28743	17.54192	17.54495	17.54687	17.54900	17.81611
1.70	16.41768	16.41839	16.41934	16.42054	16.42199	16.64195	16.64404	16.64548	16.64717	16.87621
1.80	15.67441	15.67462	15.67496	15.67545	15.67610	15.87311	15.87411	15.87488	15.87586	16.07828
1.90	15.01649	15.01628	15.01605	15.01584	15.01568	15.19991	15.19988	15.19997	15.20015	15.38630
2.00	14.41633	14.41578	14.41509	14.41429	14.41340	14.59315	14.59226	14.59173	14.59117	14.76980
2.50	11.75733	11.75638	11.75494	11.75301	11.75056	11.96562	11.96328	11.96143	11.95910	12.16708
3.00	9.36887	9.36825	9.36721	9.36572	9.36375	9.59711	9.59543	9.59394	9.59199	9.82354
3.50	7.47805	7.47767	7.47704	7.47613	7.47492	7.67407	7.67305	7.67212	7.67088	7.87436
4.00	6.19348	6.19327	6.19295	6.19249	6.19191	6.33657	6.33600	6.33551	6.33488	6.48601
5.00	4.85658	4.85669	4.85685	4.85706	4.85732	4.93137	4.93157	4.93173	4.93193	5.00846
6.00	4.10681	4.10713	4.10756	4.10809	4.10873	4.17522	4.17592	4.17643	4.17703	4.24211

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Atom      Au(2+)     Au(3+)     Au(5+)     Hg(1+)     Hg(2+)     Tl(1+)     Tl(3+)     Pb(2+)     Pb(4+)     Bi(3+)
   Z          79         79         79         80         80         81         81         82         82         83
Method        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
   0.00   77.00000   76.00000   74.00000   79.00000   78.00000   80.00000   78.00000   80.00000   78.00000   80.00000
   0.01   76.96922   75.97252   73.97761   78.96300   77.96943   79.96140   77.97262   79.96609   77.97512   79.96958
   0.02   76.87714   75.89026   73.91056   78.85243   77.87793   79.84609   77.89066   79.86470   77.90063   79.87857
   0.03   76.72447   75.75377   73.79918   78.66959   77.72621   79.65553   77.75461   79.69681   77.77691   79.72768
   0.04   76.51243   75.56397   73.64405   78.41659   77.51539   79.39205   77.56532   79.46402   77.60460   79.51811
   0.05   76.24265   75.32209   73.44594   78.09628   77.24702   79.05883   77.32393   79.16852   77.38461   79.25149

   0.06   75.91719   75.02971   73.20584   77.71214   76.92307   78.65975   77.03189   78.81305   77.11807   78.92985
   0.07   75.53849   74.68869   72.92494   77.26821   76.54583   78.19928   76.69094   78.40077   76.80632   78.55559
   0.08   75.10930   74.30118   72.60462   76.76891   76.11794   77.68232   76.30305   77.93524   76.45095   78.13146
   0.09   74.63267   73.86954   72.24639   76.21898   75.64230   77.11407   75.87045   77.42034   76.05369   77.66043
   0.10   74.11186   73.39635   71.85196   75.62330   75.12203   76.49990   75.39554   76.86013   75.61648   77.14572

   0.11   73.55030   72.88436   71.42313   74.98684   74.56045   75.84519   74.88090   76.25886   75.14139   76.59070
   0.12   72.95156   72.33642   70.96184   74.31449   73.96099   75.15525   74.32926   75.62078   74.63063   75.99885
   0.13   72.31925   71.75551   70.47011   73.61106   73.32716   74.43522   73.74343   74.95016   74.08650   75.37371
   0.14   71.65703   71.14463   69.95004   72.88112   72.66252   73.68996   73.12630   74.25119   73.51141   74.71882
   0.15   70.96850   70.50683   69.40379   72.12903   71.97059   72.92404   72.48081   73.52793   72.90781   74.03768

   0.16   70.25720   69.84515   68.83353   71.35885   71.25489   72.14167   71.80990   72.78424   72.27819   73.33372
   0.17   69.52659   69.16255   68.24148   70.57436   70.51881   71.34669   71.11650   72.02378   71.62506   72.61025
   0.18   68.77996   68.46198   67.62983   69.77901   69.76565   70.54257   70.40351   71.24998   70.95092   71.87043
   0.19   68.02047   67.74625   67.00076   68.97592   68.99857   69.73240   69.67372   70.46599   70.25825   71.11727
   0.20   67.25108   67.01809   66.35641   68.16794   68.22056   68.91894   68.92989   69.67472   69.54951   70.35360

   0.22   65.69351   65.53467   65.03025   66.54717   66.64287   67.29144   67.41049   68.08059   68.09323   68.80501
   0.24   64.12698   64.03069   63.66730   64.93373   65.05285   65.67579   65.86484   66.48553   66.60022   67.24329
   0.25   63.34562   63.27622   62.97668   64.13403   64.25868   64.87619   65.08767   65.69221   65.84520   66.46244
   0.26   62.56791   62.52257   62.28225   63.34083   63.46760   64.08367   64.31024   64.90368   65.08710   65.68383
   0.28   61.02946   61.02413   60.88821   61.77842   61.90108   62.52356   62.76160   63.34581   63.56870   64.13902
   0.30   59.52180   59.54657   59.49665   60.25380   60.36431   61.00144   61.23133   61.81990   62.05795   62.61850

   0.32   58.05246   58.09869   58.11729   58.77210   58.86557   59.52142   59.72946   60.33167   60.56577   61.12956
   0.34   56.62665   56.68706   56.75816   57.33672   57.41080   58.08617   58.26378   58.88503   59.10112   59.67749
   0.35   55.93117   55.99636   56.08824   56.63706   56.70120   57.38586   57.54638   58.17515   58.38141   58.96650
   0.36   55.24767   55.31632   55.42565   55.94963   56.00392   56.69726   56.84004   57.48251   57.67110   58.26599
   0.38   53.91727   53.98945   54.12467   54.61172   54.64715   55.35540   55.46219   56.12552   56.28107   56.89743
   0.40   52.63593   52.70806   52.85875   53.32296   53.34137   54.06060   54.13264   54.81464   54.93483   55.57315

   0.42   51.40318   51.47261   51.63026   52.08265   52.08638   52.81235   52.85252   53.54981   53.63480   54.29367
   0.44   50.21784   50.28272   50.44052   50.88953   50.88117   51.60970   51.62190   52.33042   52.38224   53.05890
   0.45   49.64242   49.70454   49.86036   50.31016   50.29673   51.02508   51.02495   51.73748   51.77388   52.45810
   0.46   49.07818   49.13731   49.29003   49.74195   49.72408   50.45136   50.44002   51.15505   51.17743   51.86823
   0.48   47.98214   48.03481   48.17858   48.63797   48.61306   49.33576   49.30547   50.02374   50.01981   50.72070
   0.50   46.92739   46.97330   47.10543   47.57545   47.54573   48.26114   48.21637   48.93359   48.90823   49.61503

   0.55   44.45526   44.48467   44.58182   45.08558   45.05183   45.74117   45.67747   46.37873   46.31895   47.02384
   0.60   42.18830   42.20366   42.26516   42.80481   42.77482   43.43372   43.36990   44.04346   43.97279   44.65771
   0.65   40.09207   40.09671   40.12742   40.69946   40.67714   41.30751   41.25485   41.89725   41.83206   42.48752
   0.70   38.13790   38.13512   38.14202   38.74047   38.72692   39.33413   39.29765   39.91127   39.86075   40.48473
   0.80   34.57303   34.56334   34.54330   35.17377   35.17489   35.75460   35.74974   36.32331   36.30862   36.88155
   0.90   31.38441   31.37451   31.34793   31.98306   31.99171   32.56106   32.57556   33.13151   33.14298   33.68897
   1.00   28.52922   28.52202   28.49967   29.11520   29.12513   29.68678   29.70726   30.25553   30.27798   30.81330

   1.10   25.99763   25.99369   25.97926   26.55553   26.56319   27.10847   27.12612   27.66342   27.68527   28.21261
   1.20   23.78740   23.78617   23.77937   24.30242   24.30659   24.82197   24.83296   25.34815   25.36337   25.87512
   1.30   21.88969   21.89024   21.88911   22.35122   22.35218   22.82485   22.82887   23.30898   23.31608   23.80020
   1.40   20.28405   20.28550   20.28777   20.68723   20.68593   21.10726   21.10587   21.54048   21.54062   21.98566
   1.50   18.93931   18.94101   18.94473   19.28496   19.28244   19.64926   19.64458   20.02801   20.02348   20.42168

   1.60   17.81727   17.81878   17.82256   18.11075   18.10790   18.42218   18.41619   18.74790   18.74106   19.08948
   1.70   16.87700   16.87809   16.88111   17.12674   17.12416   17.39188   17.38603   17.66990   17.66265   17.96295
   1.80   16.07867   16.07928   16.08114   16.29461   16.29265   16.52228   16.51749   16.76049   16.75413   17.01157
   1.90   15.38635   15.38649   15.38711   15.57865   15.57743   15.77853   15.77520   15.98603   15.98125   16.20340
   2.00   14.76958   14.76933   14.76880   14.94764   14.94712   15.12916   15.12735   15.31519   15.31221   15.50769

   2.50   12.16655   12.16562   12.16250   12.35929   12.36023   12.54408   12.54599   12.72276   12.72486   12.89534
   3.00    9.82326    9.82261    9.82007   10.04616   10.04654   10.26468   10.26553   10.47880   10.47984   10.68763
   3.50    7.87420    7.87381    7.87220    8.07778    8.07775    8.28373    8.28361    8.49139    8.49115    8.69993
   4.00    6.48590    6.48566    6.48477    6.64134    6.64130    6.80249    6.80232    6.96907    6.96872    7.14068
   5.00    5.00849    5.00855    5.00875    5.08837    5.08839    5.17142    5.17149    5.25806    5.25815    5.34861
   6.00    4.24230    4.24258    4.24342    4.30844    4.30828    4.37395    4.37367    4.43882    4.43857    4.50348
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Atom	Bi(5+)	Po(2+)	Po(4+)	Po(6+)	At(1+)	At(3+)	At(5+)	At(7+)	At(1-)	Fr(1+)
Z	83	84	84	84	85	85	85	85	85	87
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	78.00000	82.00000	80.00000	78.00000	84.00000	82.00000	80.00000	78.00000	86.00000	86.00000
0.01	77.97717	81.96113	79.97234	77.97890	83.95262	81.96539	79.97462	77.98038	85.92949	85.95168
0.02	77.90879	81.84501	79.88956	77.91567	83.81128	81.86193	79.89862	77.92158	85.72041	85.80744
0.03	77.79518	81.65315	79.75222	77.81058	83.57828	81.69068	79.77246	77.82382	85.37978	85.56941
0.04	77.63684	81.38796	79.56123	77.66405	83.25739	81.45339	79.59687	77.68747	84.91851	85.24105
0.05	77.43451	81.05272	79.31786	77.47667	82.85363	81.15241	79.37286	77.51300	84.35024	84.82704
0.06	77.18908	80.65144	79.02371	77.24920	82.37310	80.79069	79.10172	77.30107	83.69024	84.33309
0.07	76.90167	80.18875	78.68066	76.98254	81.82276	80.37167	78.78497	77.05242	82.95425	83.76579
0.08	76.57354	79.66976	78.29088	76.67774	81.21011	79.89919	78.42438	76.76794	82.15758	83.13237
0.09	76.20611	79.09985	77.85676	76.33599	80.54301	79.37741	78.02190	76.44864	81.31444	82.44050
0.10	75.80097	78.48463	77.38089	75.95862	79.82937	78.81070	77.57966	76.09563	80.43756	81.69806
0.11	75.35982	77.82972	76.86603	75.54704	79.07700	78.20360	77.09994	75.71013	79.53796	80.91294
0.12	74.88449	77.14063	76.31504	75.10280	78.29333	77.56066	76.58516	75.29344	78.62492	80.09287
0.13	74.37691	76.42270	75.73087	74.62752	77.48534	76.88640	76.03759	74.84697	77.70605	79.24524
0.14	73.83909	75.68099	75.11655	74.12292	76.65942	76.18524	75.46041	74.37217	76.78745	78.37699
0.15	73.27310	74.92018	74.47506	73.59077	75.82128	75.46142	74.85562	73.87058	75.87385	77.49450
0.16	72.68106	74.14458	73.80942	73.03290	74.97592	74.71896	74.22601	73.34379	74.96880	76.60353
0.17	72.06515	73.35806	73.12255	72.45117	74.12765	73.96160	73.57420	72.79342	74.07491	75.70915
0.18	71.42754	72.56408	72.41732	71.84749	73.28007	73.19282	72.90272	72.22114	73.19393	74.81577
0.19	70.77039	71.76564	71.69650	71.22377	72.43613	72.41576	72.21410	71.62864	72.32700	73.92711
0.20	70.09589	70.96537	70.96272	70.58193	71.59821	71.63326	71.51075	71.01761	71.47472	73.04625
0.22	68.70329	69.36783	69.46619	69.25148	69.94725	70.06171	70.06914	69.74678	69.81460	71.31728
0.24	67.26629	67.78525	67.94602	67.87111	68.33663	68.49474	68.59529	68.42216	68.21214	69.64228
0.25	66.53604	67.00262	67.18209	67.16672	67.54791	67.71695	67.85120	67.74380	67.43134	68.82724
0.26	65.80042	66.22694	66.41796	66.45516	66.77053	66.94458	67.10470	67.05688	66.66339	68.02764
0.28	64.31996	64.69890	64.89521	65.01709	65.24967	65.41979	65.61082	65.66348	65.16359	66.47468
0.30	62.83773	63.20482	63.38854	63.56925	63.77288	63.92608	64.12498	64.25369	63.70807	64.98131
0.32	61.36493	61.74689	61.90646	62.12276	62.33813	62.46702	62.65652	62.83827	62.29283	63.54355
0.34	59.91114	60.32633	60.45549	60.68740	60.94322	61.04469	61.21290	61.42693	60.91469	62.15656
0.35	59.19392	59.63031	59.74325	59.97657	60.26007	60.34767	60.50228	60.72550	60.23880	61.48057
0.36	58.48431	58.94387	59.04047	59.27156	59.58619	59.66017	59.79993	60.02821	59.57140	60.81544
0.38	57.09080	57.59990	57.66478	57.88225	58.26550	58.31391	58.42194	58.64948	58.26147	59.51569
0.40	55.73552	56.29464	56.33063	56.52516	56.98005	57.00599	57.08199	57.29695	56.98410	58.25348
0.42	54.42201	55.02816	55.03928	55.20472	55.72915	55.73626	55.78212	55.97567	55.73894	57.02572
0.44	53.15261	53.80043	53.79123	53.92417	54.51240	54.50447	54.52350	54.68959	54.52601	55.83011
0.45	52.53489	53.20105	53.18343	53.29957	53.91676	53.90269	53.90982	54.06072	53.93167	55.24382
0.46	51.92861	52.61128	52.58638	52.68570	53.32960	53.31026	53.30658	53.44168	53.34547	54.66499
0.48	50.75040	51.46036	51.42415	51.49059	52.18066	52.15321	52.13127	52.23395	52.19756	53.52927
0.50	49.61761	50.34720	50.30361	50.33928	51.06549	51.03280	50.99703	51.06760	51.08248	52.42230
0.55	46.97692	47.72466	47.67618	47.64974	48.42396	48.38785	48.33470	48.33439	48.43859	49.77868
0.60	44.58705	45.31855	45.27754	45.21407	45.98622	45.95535	45.90305	45.85353	45.99678	47.31069
0.65	42.41372	43.10881	43.08046	43.00322	43.74051	43.71858	43.67725	43.60241	43.74686	45.01609
0.70	40.42135	41.07246	41.05730	40.98373	41.67013	41.65764	41.63097	41.55111	41.67286	42.88887
0.80	36.85490	37.42778	37.43204	37.39219	37.97618	37.97808	37.97731	37.92413	37.97437	39.09085
0.90	33.69470	34.22286	34.23481	34.23223	34.75014	34.75831	34.77079	34.75768	34.74691	35.80051
1.00	30.83587	31.34828	31.35977	31.38032	31.87215	31.88059	31.89525	31.91143	31.86931	32.89719
1.10	28.23794	28.74685	28.75431	28.78205	29.27069	29.27652	29.28744	29.31611	29.26894	30.28954
1.20	25.89476	26.39746	26.40040	26.42436	26.91388	26.91651	26.92195	26.94976	26.91320	27.92407
1.30	23.81103	24.29641	24.29587	24.31094	24.79291	24.79293	24.79358	24.81320	24.79302	25.77742
1.40	21.98812	22.44316	22.44056	22.44610	22.90706	22.90545	22.90291	22.91221	22.90762	23.84334
1.50	20.41797	20.83208	20.82870	20.82654	21.25371	21.25139	21.24730	21.24747	21.25443	22.12100
1.60	19.08224	19.44941	19.44614	19.43906	19.82355	19.82119	19.81684	19.81057	19.82424	20.60733
1.70	17.95452	18.27370	18.27105	18.26175	18.59969	18.59770	18.59388	18.58416	18.60026	19.29344
1.80	17.00365	17.27804	17.27619	17.26681	17.55906	17.55761	17.55472	17.54410	17.55946	18.16400
1.90	16.19702	16.43285	16.43178	16.42373	16.67484	16.67395	16.67208	16.66237	16.67508	17.19851
2.00	15.50329	15.70850	15.70808	15.70209	15.91903	15.91862	15.91766	15.90993	15.91913	16.37332
2.50	12.89751	13.06224	13.06263	13.06475	13.22480	13.22510	13.22563	13.22754	13.22471	13.54152
3.00	10.68890	10.89101	10.89071	10.89227	11.08826	11.08809	11.08773	11.08962	11.08826	11.46361
3.50	8.69958	8.90899	8.90853	8.90811	9.11745	9.11712	9.11644	9.11600	9.11749	9.52937
4.00	7.14012	7.31708	7.31685	7.31604	7.49768	7.49749	7.49707	7.49601	7.49772	7.86904
5.00	5.34869	5.44337	5.44337	5.44341	5.54264	5.54263	5.54263	5.54259	5.54267	5.75553
6.00	4.50328	4.56846	4.56825	4.56811	4.63385	4.63371	4.63349	4.63341	4.63390	4.76714

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Atom       Ra(2+)     Ac(3+)     Th(2+)     Th(3+)     Th(4+)     Pa(3+)     Pa(4+)     Pa(5+)     U(3+)      U(4+)
   Z          88         89         90         90         90         91         91         91         92         92
Method       DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF        DHF
   STL
   0.00     86.00000   86.00000   88.00000   87.00000   86.00000   88.00000   87.00000   86.00000   89.00000   88.00000
   0.01     85.95725   85.96150   87.95334   86.96134   85.96491   87.96143   86.96491   85.96775   88.96165   87.96502
   0.02     85.82950   85.84638   87.81407   86.84573   85.85996   87.84607   86.85993   85.87125   88.84694   87.86035
   0.03     85.61827   85.65579   87.58428   86.65431   85.68605   87.65502   86.68594   85.71122   88.65692   87.68684
   0.04     85.32604   85.39162   87.26733   86.38892   85.44465   87.39005   86.44437   85.48886   88.39330   87.44588
   0.05     84.95619   85.05645   86.86774   86.05210   85.13782   87.05363   86.13721   85.20584   88.05842   87.13935

   0.06     84.51291   84.65348   86.39100   85.64702   84.76810   86.64881   85.76692   84.86423   87.65520   86.76966
   0.07     84.00107   84.18650   85.84333   85.17740   84.33851   86.17918   85.33645   84.46651   87.18711   86.33964
   0.08     83.42611   83.65978   85.23149   84.64744   83.85251   85.64881   84.84913   84.01550   86.65806   85.85251
   0.09     82.79393   83.07798   84.56255   84.06173   83.31386   85.06218   84.30866   83.51433   86.07235   85.31184
   0.10     82.11071   82.44606   83.84370   83.42519   82.72665   84.42404   83.71901   82.96640   85.43459   84.72149

   0.11     81.38278   81.76922   83.08206   82.74292   82.09517   83.73939   83.08437   82.37532   84.74961   84.08553
   0.12     80.61654   81.05273   82.28452   82.02016   81.42386   83.01335   82.40909   81.74484   84.02239   83.40820
   0.13     79.81825   80.30193   81.45766   81.26218   80.71723   82.25109   81.69763   81.07885   83.25797   82.69385
   0.14     78.99403   79.52207   80.60762   80.47422   79.97984   81.45775   80.95445   80.38126   82.46138   81.94686
   0.15     78.14965   78.71828   79.74009   79.66137   79.21616   80.63838   80.18399   79.65601   81.63757   81.17158

   0.16     77.29055   77.89547   78.86022   78.82854   78.43059   79.79786   79.39061   78.90698   80.79138   80.37233
   0.17     76.42174   77.05831   77.97268   77.98042   77.62736   78.94084   78.57852   78.13800   79.92740   79.55327
   0.18     75.54775   76.21114   77.08158   77.12138   76.81051   78.07172   77.75178   77.35274   79.05004   78.71844
   0.19     74.67263   75.35798   76.19054   76.25547   75.98384   77.19459   76.91420   76.55475   78.16339   77.87166
   0.20     73.79990   74.50244   75.30272   75.38639   75.15089   76.31320   76.06935   75.74735   77.27126   77.01654

   0.22     72.07333   72.79687   73.54705   73.65169   73.47883   74.55096   74.37085   74.11669   75.48408   75.29437
   0.24     70.38664   71.11578   71.83121   71.93943   71.81665   72.80798   72.67926   72.48301   73.71221   73.57546
   0.25     69.56217   70.28942   70.99183   71.09704   70.99489   71.94935   71.84193   71.67092   72.83795   72.72334
   0.26     68.75162   69.47449   70.16613   70.26594   70.18175   71.10161   71.01280   70.86461   71.97396   71.87880
   0.28     67.17437   67.88299   68.55811   68.64220   68.58672   69.44396   69.38505   69.27570   70.28251   70.21885
   0.30     65.65669   66.34669   67.00982   67.07464   67.03987   67.84254   67.80531   67.72666   68.64650   68.60589

   0.32     64.19732   64.86741   65.52116   65.56597   65.54581   66.30110   66.27912   66.22433   67.07071   67.04644
   0.34     62.79306   63.44434   64.09013   64.11610   64.10618   64.82039   64.80898   64.77256   65.55686   65.54388
   0.35     62.11030   62.75311   63.39523   63.41262   63.40666   64.10244   64.09503   64.06614   64.82303   64.81430
   0.36     61.43970   62.07487   62.71346   62.72295   62.72039   63.39902   63.39498   63.37272   64.10432   64.09910
   0.38     60.13272   60.75539   61.38722   61.38321   61.38624   62.03414   62.03545   62.02429   62.71082   62.71106
   0.40     58.86772   59.48182   60.10728   60.09290   60.10060   60.72202   60.72759   60.72537   61.37305   61.37739

   0.42     57.64078   58.25007   58.86955   58.84785   58.85983   59.45857   59.46791   59.47321   60.08713   60.09491
   0.44     56.44860   57.05633   57.67031   57.64402   57.66016   58.23968   58.25264   58.26452   58.84900   58.85998
   0.45     55.86468   56.47265   57.08407   57.05639   57.07461   57.64571   57.66049   57.67542   58.24660   58.25917
   0.46     55.28851   55.89727   56.50626   56.47772   56.49802   57.06145   57.07806   57.09591   57.65467   57.66886
   0.48     54.15848   54.77009   55.37463   55.34575   55.37017   55.92035   55.94067   55.96403   56.50042   56.51793
   0.50     53.05705   53.67255   54.27315   54.24543   54.27380   54.81333   54.83736   54.86581   55.38295   55.40383

   0.55     50.42288   51.04831   51.64085   51.61997   51.65656   52.17921   52.21154   52.25060   52.73225   52.76117
   0.60     47.95428   48.58406   49.16982   49.15783   49.19862   49.71515   49.75273   49.79827   50.26094   50.29572
   0.65     45.64857   46.27381   46.85257   46.84864   46.88868   47.40599   47.44450   47.49138   47.94910   47.98605
   0.70     43.50236   44.11459   44.68522   44.68728   44.72203   45.24364   45.27873   45.32185   45.78522   45.82027
   0.80     39.65773   40.22939   40.78049   40.78783   40.80407   41.33531   41.35474   41.37959   41.87075   41.89275
   0.90     36.32868   36.85994   37.39133   37.39785   37.39496   37.92996   37.93105   37.93370   38.45409   38.45872
   1.00     33.40355   33.90790   34.42408   34.42752   34.41218   34.94420   34.93195   34.91791   35.45586   35.44660

   1.10     30.78723   31.27861   31.78470   31.78519   31.76548   32.28983   32.27164   32.24970   32.79107   32.77453
   1.20     28.41739   28.90297   29.40103   29.39964   29.38165   29.89482   29.87686   29.85464   30.38756   30.36988
   1.30     26.26248   26.74146   27.22922   27.22707   27.21399   27.71207   27.69802   27.68021   28.19580   28.18102
   1.40     24.31142   24.77720   25.24885   25.24676   25.23936   25.71743   25.70861   25.69704   26.18857   26.17850
   1.50     22.56214   23.00567   23.45374   23.45213   23.44971   23.90212   23.89827   23.89276   24.35489   24.34968

   1.60     21.01312   21.42576   21.84305   21.84207   21.84327   22.26456   22.26457   22.26388   22.69241   22.69124
   1.70     19.65856   20.03398   20.41501   20.41461   20.41799   20.80386   20.80641   20.80896   21.20090   21.20258
   1.80     18.48669   18.82176   19.16362   19.16366   19.16801   19.51597   19.51985   19.52417   19.87799   19.88133
   1.90     17.48031   17.77514   18.07762   18.07792   18.08239   18.39207   18.39636   18.40131   18.71709   18.72114
   2.00     16.61837   16.87581   17.14114   17.14157   17.14563   17.41873   17.42281   17.42764   17.70707   17.71113

   2.50     13.69818   13.85540   14.01300   14.01298   14.01444   14.17309   14.17463   14.17666   14.33665   14.33830
   3.00     11.64176   11.81379   11.97843   11.97803   11.98007   12.13691   12.13878   12.14119   12.29092   12.29265
   3.50      9.73144    9.93005   10.12218   10.12181   10.12470   10.30884   10.31160   10.31504   10.49076   10.49341
   4.00      8.05855    8.24973    8.43959    8.43933    8.44189    8.62873    8.63131    8.63449    8.81716    8.81976
   5.00      5.86946    5.98849    6.11201    6.11192    6.11261    6.24012    6.24092    6.24191    6.37275    6.37366
   6.00      4.83580    4.90628    4.97900    4.97904    4.97892    5.05437    5.05428    5.05417    5.13235    5.13230
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Atom	U(5+)	U(6+)	Np(3+)	Np(4+)	Np(5+)	Np(6+)	Np(7+)	Pu(3+)	Pu(4+)	Pu(5+)
Z	92	92	93	93	93	93	93	94	94	94
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	87.00000	86.00000	90.00000	89.00000	88.00000	87.00000	86.00000	91.00000	90.00000	89.00000
0.01	86.96779	85.97016	89.96195	88.96520	87.96789	86.97020	85.97224	90.96230	89.96544	88.96805
0.02	86.87138	85.88083	89.84814	88.86107	87.87179	86.88101	85.88912	90.84953	89.86200	88.87240
0.03	86.71149	85.73263	89.65955	88.68842	87.71238	86.73300	85.75115	90.66262	89.69047	88.71372
0.04	86.48927	85.52653	89.39781	88.44858	87.49077	86.52713	85.55917	90.40312	89.45211	88.49307
0.05	86.20632	85.26392	89.06517	88.14337	87.20851	86.26472	85.31431	90.07318	89.14867	88.21194
0.06	85.86465	84.94651	88.66442	87.77508	86.86752	85.94745	85.01805	89.67544	88.78235	87.87217
0.07	85.46666	84.57637	88.19886	87.34644	86.47011	85.57729	84.67210	89.21309	88.35576	87.47600
0.08	85.01508	84.15586	87.67226	86.86055	86.01894	85.15653	84.27849	88.68969	87.87189	87.02597
0.09	84.51295	83.68761	87.08873	86.32086	85.51694	84.68773	83.83943	88.10922	87.33405	86.52492
0.10	83.96358	83.17449	86.45271	85.73109	84.96730	84.17367	83.35739	87.47592	86.74583	85.97593
0.11	83.37046	82.61956	85.76887	85.09519	84.37342	83.61732	82.83498	86.79430	86.11104	85.38231
0.12	82.73728	82.02603	85.04202	84.41728	83.73890	83.02183	82.27499	86.06900	85.43366	84.74751
0.13	82.06782	81.39726	84.27706	83.70157	83.06740	82.39045	81.68032	85.30476	84.71780	84.07513
0.14	81.36593	80.73665	83.47889	82.95234	82.36270	81.72651	81.05395	84.50636	83.96762	83.36883
0.15	80.63548	80.04765	82.65237	82.17387	81.62859	81.03341	80.39892	83.67853	83.18728	82.63232
0.16	79.88032	79.33371	81.80223	81.37038	80.86884	80.31454	79.71828	82.82589	82.38094	81.86930
0.17	79.10422	78.59825	80.93303	80.54600	80.08719	79.57326	79.01510	81.95296	81.55264	81.08344
0.18	78.31085	77.84460	80.04912	79.70471	79.28726	78.81290	78.29240	81.06402	80.70631	80.27832
0.19	77.50374	77.07602	79.15461	78.85032	78.47256	78.03666	77.55313	80.16315	79.84575	79.45741
0.20	76.68624	76.29562	78.25331	77.98644	77.64646	77.24767	76.80017	79.25417	78.97453	78.62406
0.22	75.03255	74.71102	76.44408	76.24345	75.97255	75.64315	75.26414	77.42575	77.21344	76.93257
0.24	73.37246	73.11239	74.64572	74.49965	74.28850	74.02114	73.70483	75.60348	75.44723	75.22700
0.25	72.54608	72.31370	73.75680	73.63374	73.44889	73.20958	72.92221	74.70104	74.56865	74.37527
0.26	71.72488	71.51815	72.87738	72.77465	72.61373	72.40048	72.14034	73.80720	73.69603	73.52717
0.28	70.10483	69.94337	71.15323	71.08376	70.96394	70.79683	70.58602	72.05198	71.97584	71.84935
0.30	68.52351	68.39976	69.48297	69.43814	69.35114	69.22260	69.05435	70.34849	70.29868	70.20628
0.32	66.98869	66.89583	67.87245	67.84528	67.78392	67.68708	67.55500	68.70360	68.67291	68.60733
0.34	65.50503	65.43722	66.32433	66.30946	66.26782	66.19667	66.09499	67.12093	67.10372	67.05884
0.35	64.78315	64.72598	65.57381	65.56356	65.52994	65.46969	65.38126	66.35334	66.34122	66.30478
0.36	64.07469	64.02708	64.83882	64.83238	64.80575	64.75527	64.67892	65.60155	65.59363	65.56454
0.38	62.69778	62.66649	63.41435	63.41371	63.39853	63.36465	63.30934	64.14461	64.14303	64.12592
0.40	61.37291	61.35495	62.04809	62.05163	62.04534	62.02487	61.98707	62.74786	62.75073	62.74280
0.42	60.09763	60.09075	60.73650	60.74333	60.74416	60.73470	60.71157	61.40818	61.41438	61.41367
0.44	58.86889	58.87143	59.47569	59.48545	59.49224	59.49199	59.48129	60.12194	60.13094	60.13611
0.45	58.27093	58.27769	58.86308	58.87427	58.88375	58.88760	58.88243	59.49768	59.50798	59.51576
0.46	57.68332	57.69405	58.26170	58.27432	58.28635	58.29402	58.29399	58.88534	58.89694	58.90717
0.48	56.53750	56.55550	57.09075	57.10631	57.12312	57.13774	57.14702	57.69459	57.70884	57.72359
0.50	55.42818	55.45269	55.95933	55.97794	55.99921	56.02006	56.03753	56.54611	56.56311	56.58206
0.55	52.79588	52.83379	53.28422	53.31044	53.34164	53.37546	53.40953	53.83921	53.86329	53.89167
0.60	50.33755	50.38444	50.79975	50.83209	50.87070	50.91375	50.95943	51.33541	51.36565	51.40149
0.65	48.03062	48.08131	48.48146	48.51686	48.55918	48.60704	48.65909	49.00621	49.04012	49.08034
0.70	45.86285	45.91198	46.31425	46.34899	46.39075	46.43856	46.49152	46.83296	46.86720	46.90797
0.80	41.92031	41.95341	42.39421	42.41826	42.44790	42.48299	42.52345	42.90605	42.93172	42.96293
0.90	38.46556	38.47523	38.96915	38.97694	38.98744	39.00111	39.01845	39.47427	39.48489	39.49857
1.00	35.43632	35.42585	35.96120	35.95482	35.94810	35.94175	35.93649	36.45890	36.45529	36.45193
1.10	32.75486	32.73277	33.28782	33.27307	33.25578	33.23660	33.21616	33.77886	33.76599	33.75114
1.20	30.34827	30.32318	30.87713	30.85997	30.83924	30.81540	30.78882	31.36250	31.34607	31.32645
1.30	28.16253	28.14054	28.67770	28.66243	28.64357	28.62134	28.59589	29.15691	29.14138	29.12242
1.40	26.16553	26.14967	26.65967	26.64852	26.63440	26.61734	26.59728	27.12090	27.11785	27.10281
1.50	24.34257	24.33342	24.80990	24.80342	24.79485	24.78408	24.77097	25.26625	25.25860	25.24872
1.60	22.68910	22.68578	23.12504	23.12269	23.11915	23.11422	23.10772	23.56148	23.55799	23.55309
1.70	21.20401	21.20498	21.60518	21.60594	21.60624	21.60587	21.60463	22.01572	22.01554	22.01468
1.80	19.88493	19.88858	20.24930	20.25204	20.25485	20.25753	20.25992	20.62899	20.63106	20.63303
1.90	18.72572	18.73068	19.05279	19.05652	19.06066	19.06504	19.06952	19.39842	19.40177	19.40538
2.00	17.71587	17.72114	18.00668	18.01066	18.01523	18.02025	18.02561	18.31705	18.32088	18.32521
2.50	14.34044	14.34306	14.50490	14.50669	14.50897	14.51172	14.51494	14.67852	14.68046	14.68289
3.00	12.29488	12.29760	12.44100	12.44261	12.44470	12.44724	12.45022	12.58768	12.58920	12.59116
3.50	10.49669	10.50055	10.66771	10.67024	10.67337	10.67705	10.68125	10.83939	10.84180	10.84478
4.00	8.82295	8.82666	9.00437	9.00698	9.01016	9.01385	9.01804	9.18957	9.19217	9.19533
5.00	6.37477	6.37608	6.50988	6.51090	6.51214	6.51359	6.51522	6.65102	6.65214	6.65351
6.00	5.13223	5.13216	5.21347	5.21346	5.21345	5.21344	5.21342	5.29771	5.29775	5.29779

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Atom Z Method STL	Pu(6+) 94 DHF	Pu(7+) 94 DHF	Am(2+) 95 DHF	Am(3+) 95 DHF	Am(4+) 95 DHF	Am(5+) 95 DHF	Am(6+) 95 DHF	Cm(3+) 96 DHF	Cm(4+) 96 DHF	Bk(3+) 97 DHF
0.00	88.00000	87.00000	93.00000	92.00000	91.00000	90.00000	89.00000	93.00000	92.00000	94.00000
0.01	87.97030	86.97228	92.95885	91.96269	90.96571	89.96824	88.97043	92.96309	91.96600	93.96350
0.02	87.88138	86.88930	92.83578	91.85104	90.86308	89.87317	88.88190	92.85264	91.86425	93.85428
0.03	87.73380	86.75152	92.63195	91.66597	90.69285	89.71540	88.73494	92.66951	91.69545	93.67315
0.04	87.52849	86.55977	92.34926	91.40894	90.45623	89.49597	88.53045	92.41509	91.46076	93.42144
0.05	87.26672	86.31514	91.99030	91.08199	90.15490	89.21630	88.26964	92.09133	91.16178	93.10100
0.06	86.95009	86.01905	91.55830	90.68766	89.79096	88.87818	87.95406	91.70065	90.80053	92.71414
0.07	86.58052	85.67318	91.05707	90.22895	89.36691	88.48374	87.58557	91.24592	90.37939	92.26361
0.08	86.16022	85.27945	90.49090	89.70931	88.88563	88.03543	87.16630	90.73042	89.90113	91.75254
0.09	85.69166	84.84004	89.86447	89.13253	88.35030	87.53598	86.69861	90.15779	89.36881	91.18440
0.10	85.17754	84.35733	89.18278	88.50268	87.76436	86.98837	86.18513	89.53194	88.78573	90.56295
0.11	84.62073	83.83386	88.45104	87.82410	87.13150	86.39580	85.62864	88.85702	88.15545	89.89219
0.12	84.02429	83.27234	87.67460	87.10126	86.45557	85.76161	85.03210	88.13736	87.48169	89.17627
0.13	83.39138	82.67560	86.85882	86.33375	85.74054	85.08929	84.39859	87.37739	86.76829	88.41948
0.14	82.72528	82.04655	86.00905	85.54120	84.99045	84.38240	83.73129	86.58158	86.01916	87.62614
0.15	82.02928	81.38816	85.13054	84.71322	84.20937	83.64457	83.03343	85.75442	85.23827	86.80061
0.16	81.30673	80.70345	84.22834	83.85933	83.40134	82.87940	82.30827	84.90032	84.42956	85.94720
0.17	80.56092	79.99542	83.30729	82.98394	82.57033	82.09049	81.55906	84.02360	83.59691	85.07011
0.18	79.79514	79.26705	82.37196	82.09130	81.72024	81.28138	80.78901	83.12843	82.74414	84.17344
0.19	79.01257	78.52127	81.42663	81.18544	80.85478	80.45548	80.00128	82.21880	81.87493	83.26112
0.20	78.21631	77.76094	80.47524	80.27017	79.97752	79.61613	79.19893	81.29849	80.99281	82.33689
0.22	76.59442	76.20758	78.56838	78.42529	78.20090	77.90953	77.56207	79.43970	79.20305	80.46654
0.24	74.95142	74.62760	76.67607	76.58170	76.41473	76.18480	75.90038	77.57727	77.39927	78.58764
0.25	74.12811	73.83345	75.74159	75.66693	75.52463	75.32206	75.06640	76.65138	76.49877	77.65179
0.26	73.30647	73.03934	74.81754	74.75978	74.63953	74.46207	74.23326	75.73206	75.60229	76.72142
0.28	71.67571	71.45858	73.00694	72.97540	72.89193	72.75809	72.57726	73.92057	73.82925	74.88492
0.30	70.07218	69.89834	71.25392	71.24012	71.18467	71.08622	70.94593	72.15518	72.09354	73.09124
0.32	68.50585	68.36893	69.56433	69.56175	69.52696	69.45657	69.34990	70.44456	70.40513	71.34982
0.34	66.98388	66.87804	67.94093	67.94484	67.92482	67.87624	67.79701	68.79415	68.77083	69.66694
0.35	66.24107	66.14878	67.15426	67.16012	67.14572	67.10606	67.03850	67.99247	67.97536	68.84865
0.36	65.51091	65.43096	66.38413	66.39132	66.38158	66.34970	66.29260	67.20671	67.19477	68.04615
0.38	64.08938	64.03090	64.89255	64.90109	64.89840	64.87918	64.83980	65.68289	65.67882	66.48886
0.40	62.71997	62.67927	63.46363	63.47252	63.47470	63.46513	63.43991	64.22172	64.22308	64.99477
0.42	61.40195	61.37605	62.09407	62.10298	62.10868	62.10657	62.09275	62.82110	62.82629	63.56231
0.44	60.13358	60.12010	60.78013	60.78919	60.79767	60.80153	60.79701	61.47816	61.48625	62.18907
0.45	59.51727	59.50927	60.14282	60.15209	60.16182	60.16827	60.16779	60.82729	60.83663	61.52374
0.46	58.91242	58.90950	59.51799	59.52756	59.53851	59.54735	59.55059	60.18958	60.20010	60.87207
0.48	57.73559	57.74178	58.30387	58.31440	58.32777	58.34098	58.35086	58.95186	58.96465	59.60804
0.50	56.60004	56.61422	57.13422	57.14615	57.16201	57.17921	57.19491	57.76150	57.77658	58.39361
0.55	53.92216	53.95249	54.38390	54.40063	54.42303	54.44918	54.47696	54.97125	54.99235	55.55321
0.60	51.44125	51.48319	51.84964	51.87142	51.89986	51.93335	51.97031	52.41077	52.43770	52.95599
0.65	49.12557	49.17452	49.50123	49.52651	49.55901	49.59730	49.64014	50.04520	50.07642	50.56485
0.70	46.95433	47.00539	47.31760	47.34388	47.37749	47.41720	47.46208	47.84945	47.88238	48.35199
0.80	42.99945	43.04110	43.38644	43.40733	43.43426	43.46663	43.50413	43.89932	43.92722	44.38340
0.90	39.51568	39.53658	39.95954	39.96938	39.98249	39.99895	40.01899	40.45467	40.46998	40.93056
1.00	36.44942	36.44838	36.94951	36.94832	36.94735	36.94712	36.94815	37.42900	37.43053	37.90069
1.10	33.73491	33.71788	34.27218	34.26338	34.25246	34.24007	34.22677	34.74067	34.73174	35.21014
1.20	31.30410	31.27939	31.85504	31.84292	31.82741	31.80910	31.78843	32.31764	32.30321	32.78595
1.30	29.10028	29.07513	29.64469	29.63275	29.61717	29.59838	29.57660	30.10450	30.08908	30.57140
1.40	27.08483	27.06390	27.60818	27.59861	27.58584	27.57010	27.55147	28.06506	28.05176	28.52847
1.50	25.23652	25.22189	25.72959	25.72328	25.71457	25.70352	25.69008	26.18020	26.17056	26.63619
1.60	23.54664	23.53845	24.00413	24.00104	23.99644	23.99026	23.98238	24.44290	24.43725	24.88617
1.70	22.01296	22.01020	22.43226	22.43183	22.43068	22.42867	22.42562	22.85269	22.85058	23.27741
1.80	20.63469	20.63590	21.01500	21.01645	21.01781	21.01888	21.01948	21.41094	21.41154	21.81158
1.90	19.40910	19.41278	19.75095	19.75353	19.75643	19.75944	19.76243	20.11752	20.11990	20.48961
2.00	18.32989	18.33482	18.63490	18.63796	18.64159	18.64560	18.64986	18.96902	18.97236	19.30961
2.50	14.68580	14.68917	14.85694	14.85851	14.86061	14.86320	14.86627	15.04564	15.04791	15.24047
3.00	12.59355	12.59638	12.73089	12.73190	12.73335	12.73522	12.73750	12.87453	12.87593	13.01633
3.50	10.84827	10.85227	11.00429	11.00601	11.00830	11.01112	11.01444	11.16772	11.16990	11.32465
4.00	9.19900	9.20315	9.37049	9.37247	9.37506	9.37819	9.38181	9.55270	9.55527	9.72983
5.00	6.65509	6.65687	6.79510	6.79605	6.79728	6.79877	6.80048	6.94472	6.94606	7.09661
6.00	5.29785	5.29791	5.38534	5.38541	5.38551	5.38562	5.38574	5.47680	5.47695	5.57191

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Atom	Bk(4+)	Cf(2+)	Cf(3+)	Cf(4+)	Es(2+)	Es(3+)	Fm(2+)	Fm(3+)	Md(2+)	Md(3+)
Z	97	98	98	98	99	99	100	100	101	101
Method	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF	DHF
STL										
0.00	93.00000	96.00000	95.00000	94.00000	97.00000	96.00000	98.00000	97.00000	99.00000	98.00000
0.01	92.96632	95.96055	94.96392	93.96665	96.96110	95.96435	97.96163	96.96477	98.96216	97.96519
0.02	92.86550	95.84251	94.85595	93.86680	96.84469	95.85763	97.84683	96.85931	98.84892	97.86098
0.03	92.69822	95.64687	94.67685	93.70111	96.65171	95.68059	97.65646	96.68432	98.66112	97.68804
0.04	92.46559	95.37523	94.42791	93.47063	96.38368	95.43443	97.39198	96.44097	98.40013	97.44748
0.05	92.16914	95.02977	94.11087	93.17682	96.04267	95.12084	97.05536	96.13085	98.06783	97.14083
0.06	91.81078	94.61326	93.72795	92.82154	95.63131	94.74193	96.64910	95.75597	97.66660	96.77002
0.07	91.39284	94.12894	93.28176	92.40698	95.15268	94.30019	96.17612	95.31874	97.19924	96.33732
0.08	90.91793	93.58050	92.77531	91.93567	94.61029	93.79849	95.63980	94.82190	96.66895	95.84539
0.09	90.38900	92.97198	92.21192	91.41043	94.00801	93.24003	95.04381	94.26849	96.07926	95.29713
0.10	89.80923	92.30775	91.59519	90.83433	93.35002	92.62825	94.39215	93.66185	95.43401	94.69575
0.11	89.18205	91.59239	90.92896	90.21066	92.64069	91.96685	93.68904	93.00551	94.73723	94.04464
0.12	88.51104	90.83063	90.21724	89.54288	91.88459	91.25968	92.93885	92.30318	93.99312	93.34739
0.13	87.79992	90.02729	89.46415	88.83457	91.08636	90.51073	92.14605	91.55871	93.20602	92.60769
0.14	87.05248	89.18722	88.67389	88.08942	90.25068	89.72405	91.31517	90.77602	92.38027	91.82934
0.15	86.27257	88.31520	87.85067	87.31116	89.38220	88.90373	90.45071	89.95908	91.52026	91.01619
0.16	85.46402	87.41595	86.99869	86.50352	88.48549	88.05384	89.55713	89.11183	90.63030	90.17206
0.17	84.63065	86.49401	86.12207	85.67022	87.56500	87.17839	88.63875	88.23819	89.71462	89.30077
0.18	83.77618	85.55376	85.22480	84.81490	86.62500	86.28131	87.69978	87.34199	88.77732	88.40606
0.19	82.90424	84.59932	84.31075	83.94113	85.66958	85.36638	86.74420	86.42694	87.82232	87.49156
0.20	82.01830	83.63459	83.38361	83.05233	84.70259	84.43725	85.77584	85.49663	86.85339	86.56079
0.22	80.21759	81.68850	81.50383	81.24267	82.74804	82.54999	83.81478	83.60367	84.88760	84.66374
0.24	78.39842	79.74102	79.61070	79.41018	80.78695	80.64469	81.84219	81.68811	82.90543	82.73970
0.25	77.48862	78.77348	78.66598	78.49212	79.81076	79.69217	80.85844	80.72877	81.91512	81.77446
0.26	76.58183	77.81307	77.72567	77.57604	78.84057	78.74295	79.87953	79.77164	80.92851	80.81035
0.28	74.78534	75.92104	75.86625	75.75809	76.92581	76.86264	77.94415	77.87241	78.97453	78.89409
0.30	73.02295	74.07717	74.04614	73.97081	75.05559	75.01800	76.04955	76.00511	77.05748	77.00595
0.32	71.30528	72.29001	72.27551	72.22543	73.23920	73.21984	74.20570	74.18110	75.18794	75.15781
0.34	69.63988	70.56499	70.56140	70.53018	71.48286	71.47587	72.41952	72.40875	73.37347	73.35859
0.35	68.82840	69.72677	69.72697	69.70319	70.62843	70.62588	71.54950	71.54382	72.48855	72.47939
0.36	68.03163	68.90500	68.90812	68.89063	69.79019	69.79114	70.69535	70.69376	71.61909	71.61462
0.38	66.48312	67.31086	67.31780	67.31006	68.16275	68.16848	69.03544	69.03962	69.92770	69.93001
0.40	64.99510	65.78191	65.79080	65.78987	66.60050	66.60887	67.44036	67.44794	68.30046	68.30697
0.42	63.56690	64.31635	64.32613	64.32997	65.10219	65.11191	65.90943	65.91889	66.73726	66.74622
0.44	62.19678	62.91164	62.92184	62.92911	63.66575	63.67615	64.44104	64.45151	65.23695	65.24732
0.45	61.53275	62.23118	62.24154	62.25021	62.96992	62.98055	63.72962	63.74042	64.50982	64.52067
0.46	60.88227	61.56479	61.57533	61.58524	62.28854	62.29939	63.03295	63.04404	63.79769	63.80892
0.48	59.62045	60.27256	60.28361	60.29575	60.96760	60.97895	61.68249	61.69413	62.41717	62.42905
0.50	58.40817	59.03166	59.04352	59.05772	59.69983	59.71189	60.38680	60.39910	61.09277	61.10532
0.55	55.57334	56.13308	56.14827	56.16767	56.74278	56.75778	57.36783	57.38277	58.00903	58.02401
0.60	52.98167	53.48975	53.50925	53.53392	54.05337	54.07239	54.62825	54.64691	55.21566	55.23407
0.65	50.59491	51.06441	51.08775	51.11680	51.59319	51.61599	52.12901	52.15135	52.67344	52.69541
0.70	48.38421	48.82814	48.85369	48.88521	49.33140	49.35663	49.83779	49.86270	50.34900	50.37361
0.80	44.41202	44.83753	44.86111	44.89027	45.30995	45.33409	45.77933	45.80391	46.24727	46.27217
0.90	40.94781	41.38270	41.39776	41.41670	41.84074	41.85718	42.29216	42.30984	42.73809	42.75686
1.00	37.90457	38.35893	38.36343	38.36949	38.81127	38.81750	39.25547	39.26333	39.69214	39.70153
1.10	35.20320	35.67577	35.67142	35.66646	36.12718	36.12437	36.57023	36.56896	37.00512	37.00535
1.20	32.77273	33.25705	33.24728	33.23537	33.70999	33.70123	34.15514	34.14747	34.59240	34.58587
1.30	30.55633	31.04447	31.03278	31.01822	31.49942	31.48812	31.94768	31.93689	32.38893	32.37876
1.40	28.51481	28.99903	28.98812	28.97426	29.45444	29.44336	29.90469	29.89357	30.34927	30.33824
1.50	26.62575	27.09902	27.09046	27.07934	27.55140	27.54229	28.00051	27.99097	28.44572	28.43585
1.60	24.87954	25.33562	25.33002	25.32249	25.78000	25.77367	26.22330	26.21631	26.66480	26.65722
1.70	23.27435	23.70784	23.70511	23.70112	24.13847	24.13498	24.57039	24.56618	25.00280	24.99790
1.80	21.81139	22.21789	22.21753	22.21653	22.62902	22.62799	23.04380	23.04211	23.46142	23.45907
1.90	20.49142	20.86769	20.86904	20.87024	21.25427	21.25511	21.64669	21.64700	22.04418	22.04392
2.00	19.31261	19.65672	19.65913	19.66173	20.01493	20.01700	20.38081	20.38251	20.75370	20.75499
2.50	15.24290	15.44146	15.44351	15.44610	15.65306	15.65526	15.87368	15.87602	16.10363	16.10609
3.00	13.01770	13.15715	13.15813	13.15949	13.29982	13.30083	13.44418	13.44522	13.59106	13.59215
3.50	11.32671	11.47559	11.47707	11.47902	11.62397	11.62538	11.76862	11.76995	11.91005	11.91131
4.00	9.73235	9.90157	9.90352	9.90599	10.07170	10.07361	10.23803	10.23991	10.40053	10.40235
5.00	7.09805	7.25011	7.25133	7.25287	7.40727	7.40857	7.56651	7.56789	7.72750	7.72895
6.00	5.57212	5.67059	5.67081	5.67109	5.77336	5.77365	5.88006	5.88040	5.99072	5.99112

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Atom      No(2+)      No(3+)      Lr(3+)      Rf(4+)      Db(5+)      Sg(6+)      Bh(7+)      Hs(8+)      Cn(2+)
    Z        102         102         103         104         105         106         107         108         112
Method       DHF         DHF         DHF         DHF         DHF         DHF         DHF         DHF         DHF
  STL
 0.00  100.00000    99.00000   100.00000   100.00000   100.00000   100.00000   100.00000   100.00000   110.00000
 0.01   99.96268    98.96560    99.96602    99.96870    99.97094    99.97286    99.97454    99.97603   109.95604
 0.02   99.85097    98.86263    99.86427    99.87495    99.88389    99.89157    99.89827    99.90421   109.82456
 0.03   99.66568    98.69173    99.69538    99.71926    99.73927    99.75646    99.77149    99.78480   109.60668
 0.04   99.40811    98.45395    99.46036    99.50244    99.53774    99.56811    99.59467    99.61821   109.30431
 0.05   99.08005    98.15076    99.16060    99.22562    99.28027    99.32732    99.36852    99.40505   108.92000

 0.06   98.68378    97.78400    98.79787    98.89024    98.96802    99.03509    99.09388    99.14605   108.45699
 0.07   98.22197    97.35585    98.37427    98.49801    98.60245    98.69265    98.77181    98.84214   107.91903
 0.08   97.69768    96.86886    97.89222    98.05092    98.18520    98.30139    98.40353    98.49436   107.31043
 0.09   97.11429    96.32581    97.35442    97.55117    97.71813    97.86292    97.99039    98.10391   106.63585
 0.10   96.47547    95.72978    96.76381    97.00120    97.20331    97.37898    97.53392    97.67212   105.90032

 0.11   95.78509    95.08404    96.12353    96.40364    96.64294    96.85148    97.03578    97.20043   105.10906
 0.12   95.04722    94.39204    95.43692    95.76128    96.03941    96.28247    96.49775    96.69041   104.26745
 0.13   94.26601    93.65734    94.70741    95.07701    95.39521    95.67410    95.92170    96.14371   103.38095
 0.14   93.44567    92.88363    93.93857    94.35387    94.71294    95.02865    95.30963    95.56210   102.45496
 0.15   92.59045    92.07461    93.13398    93.59494    93.99527    94.34844    94.66360    94.94738   101.49482

 0.16   91.70454    91.23401    92.29726    92.80337    93.24496    93.63590    93.98574    94.30146   100.50571
 0.17   90.79206    90.36554    91.43202    91.98230    92.46476    92.89346    93.27821    93.62628    99.49260
 0.18   89.85700    89.47285    90.54182    91.13489    91.65748    92.12362    92.54325    92.92383    98.46021
 0.19   88.90323    88.55950    89.63014    90.26425    90.82590    91.32886    91.78308    92.19611    97.41298
 0.20   87.93443    87.62893    88.70036    89.37343    89.97277    90.51167    90.99996    91.44517    96.35504

 0.22   85.96551    85.72925    86.79936    87.54314    88.21268    88.81984    89.37376    89.88171    94.22192
 0.24   83.97555    83.79834    84.86310    85.66666    86.39814    87.06735    87.68230    88.24961    92.08729
 0.25   82.97961    82.82807    83.88860    84.71765    85.47662    86.17412    86.81743    87.41277    91.02623
 0.26   81.98625    81.85787    82.91313    83.76470    84.54869    85.27247    85.94255    86.56461    89.97235
 0.28   80.01559    79.92636    80.96806    81.85569    82.68215    83.45217    84.17052    84.84174    87.89340
 0.30   78.07796    78.01916    79.04349    79.95564    80.81439    81.62188    82.38104    83.09511    85.86237

 0.32   76.18448    76.14856    77.15209    78.07801    78.95918    79.79531    80.58753    81.33772    83.88751
 0.34   74.34331    74.32401    75.30375    76.23386    77.12820    77.98442    78.80194    79.58131    81.97399
 0.35   73.44419    73.43125    74.39815    75.32715    76.22488    77.08808    77.91542    78.70679    81.04118
 0.36   72.56009    72.55241    73.50591    74.43192    75.33106    76.19932    77.03465    77.83631    80.12457
 0.38   70.83830    70.83844    71.76376    72.67879    73.57542    74.44841    75.29446    76.11177    78.34015
 0.40   69.17973    69.18489    70.08065    70.97922    71.86714    72.73836    73.58869    74.41539    76.62025

 0.42   67.58477    67.59302    68.45836    69.33631    70.21044    71.07434    71.92320    72.75356    74.96339
 0.44   66.05277    66.06288    66.89743    67.75176    68.60814    69.46011    70.30251    71.13141    73.36748
 0.45   65.30996    65.32070    66.13985    66.98160    67.82793    68.67249    69.51004    70.33649    72.59160
 0.46   64.58231    64.59356    65.39737    66.22618    67.06185    67.89818    68.72993    69.55290    71.82999
 0.48   63.17141    63.18346    63.95698    64.75922    65.57215    66.39002    67.20772    68.02095    70.34817
 0.50   61.81773    61.83052    62.57450    63.34988    64.13882    64.93619    65.73717    66.53754    68.91922

 0.55   58.66694    58.68201    59.35712    60.06746    60.79511    61.53669    62.28856    63.04722    65.56011
 0.60   55.81660    55.83486    56.45007    57.10232    57.77208    58.45756    59.15650    59.86646    62.47419
 0.65   53.22784    53.24950    53.81475    54.41776    55.03653    55.67041    56.31831    56.97884    59.62780
 0.70   50.86656    50.89089    51.41589    51.97831    52.55393    53.14279    53.74462    54.35888    56.99409
 0.80   46.71523    46.74037    47.20995    47.71235    48.22280    48.74182    49.26987    49.80734    52.28495
 0.90   43.17967    43.19939    43.63860    44.10095    44.56727    45.03819    45.51433    45.99629    48.22327
 1.00   40.12196    40.13277    40.55782    40.99360    41.43014    41.86821    42.30849    42.75165    44.71810

 1.10   37.43210    37.43381    37.85471    38.27424    38.69178    39.10829    39.52454    39.94129    41.68824
 1.20   35.02170    35.01636    35.43898    35.85073    36.25814    36.66226    37.06393    37.46399    39.05412
 1.30   32.82287    32.81340    33.24063    33.65115    34.05553    34.45473    34.84960    35.24099    36.73861
 1.40   30.78772    30.77689    31.20914    31.62256    32.02878    32.42855    32.82256    33.21158    34.67119
 1.50   28.88642    28.87633    29.31187    29.72958    30.13993    30.54332    30.94018    31.33108    32.79204

 1.60   27.10377    27.09569    27.53104    27.95178    28.36588    28.77338    29.17438    29.56913    31.05447
 1.70   25.43490    25.42936    25.85981    26.28014    26.69538    27.10516    27.50924    27.90755    29.42532
 1.80   23.88105    23.87805    24.29824    24.71330    25.12540    25.53385    25.93807    26.33767    27.88378
 1.90   22.44590    22.44508    22.84964    23.25394    23.65775    24.06014    24.46027    24.85750    26.41906
 2.00   21.13282    21.13366    21.51778    21.90594    22.29616    22.68737    23.07857    23.46892    25.02773

 2.50   16.34303    16.34558    16.59454    16.85604    17.12718    17.40756    17.69657    17.99367    19.26269
 3.00   13.74122    13.74237    13.89660    14.05720    14.22367    14.39662    14.57648    14.76366    15.58806
 3.50   12.04877    12.04997    12.18646    12.32282    12.45850    12.59418    12.73049    12.86816    13.44497
 4.00   10.55913    10.56088    10.71554    10.86841    11.01787    11.16409    11.30731    11.44787    11.99828
 5.00    7.88979     7.89131     8.05455     8.22022     8.38638     8.55265     8.71857     8.88382     9.54208
 6.00    6.10529     6.10576     6.22423     6.34717     6.47402     6.60466     6.73887     6.87648     7.46137
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Figure S1. Differences between the X-ray scattering factors calculated in this work and the previous studies plotted for each atom as a function of $\sin\theta/\lambda$ using the Doyle & Turner (1968) grid (common to all the studies). The previous studies are abbreviated as follows: DT – Doyle & Turner (1968), CW – Cromer & Waber (1968), CM – Cromer & Mann (1968), FOT – Fox, O'Keefe & Tabbernor (1989), TS – Thakkar & Smith (1992), RRG – Rez, Rez, & Grant (1994), WSBJ – Wang, Smith, Bunge & Jáiregui (1996), and MC – Macchi & Coppens (2001).

1) Li$^+$

2) Be^{2+}

3) C$_{val}$

4) O$^-$

5) F⁻

6) Na⁺

7) Mg²⁺

8) Al³⁺

9) Si_val

10) Si⁴⁺
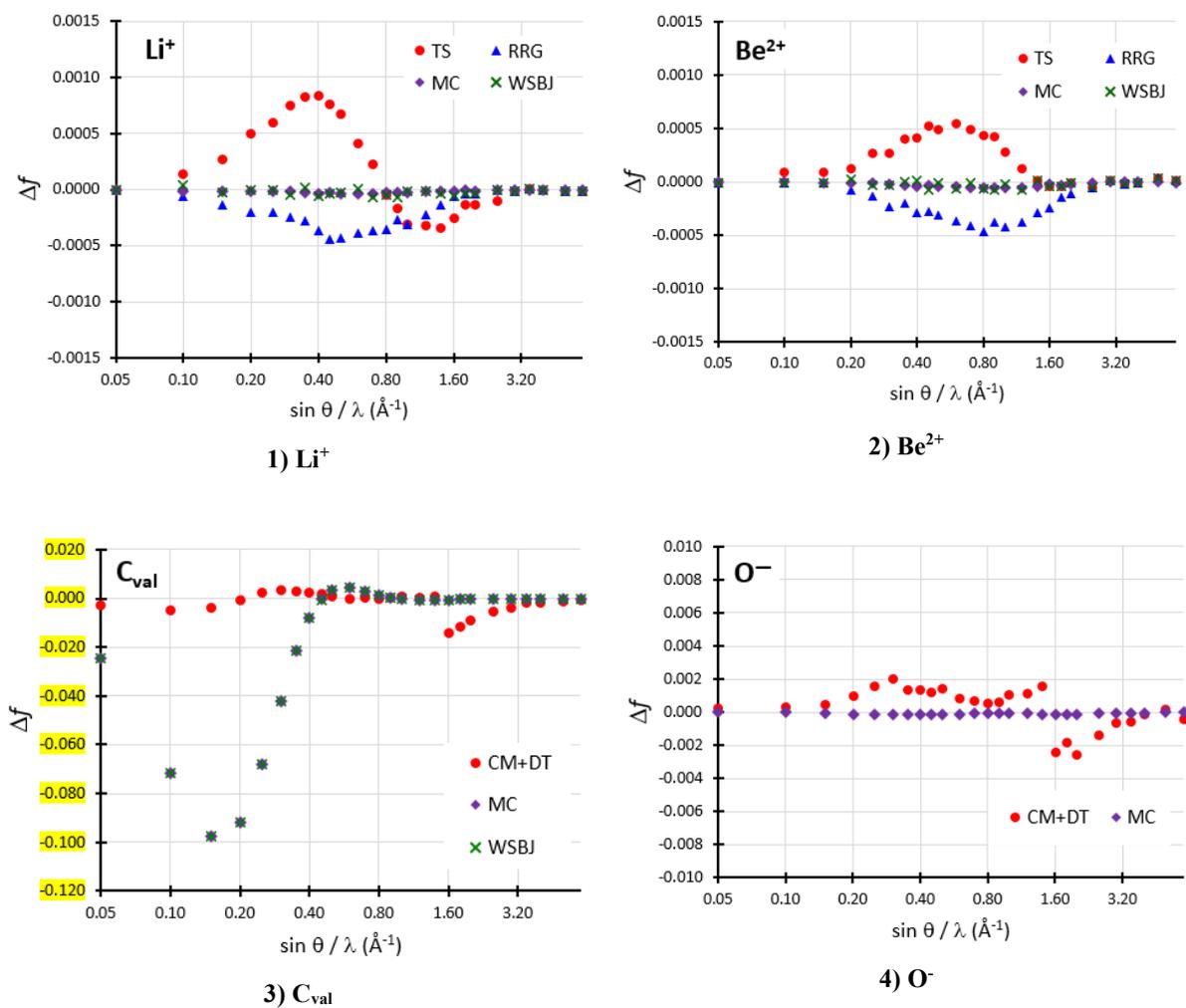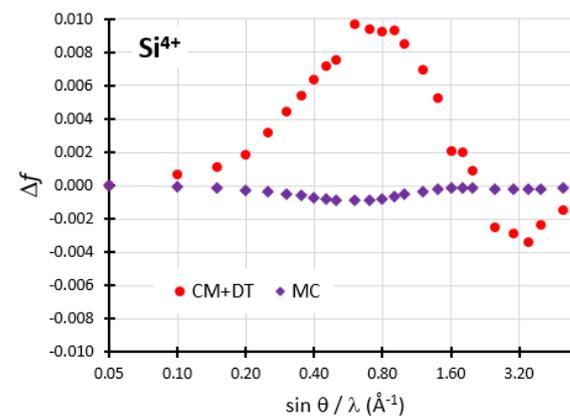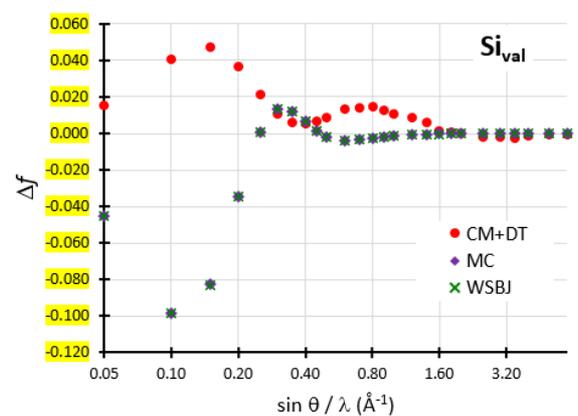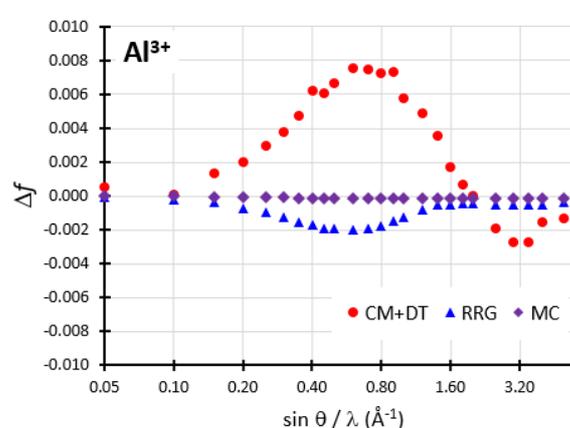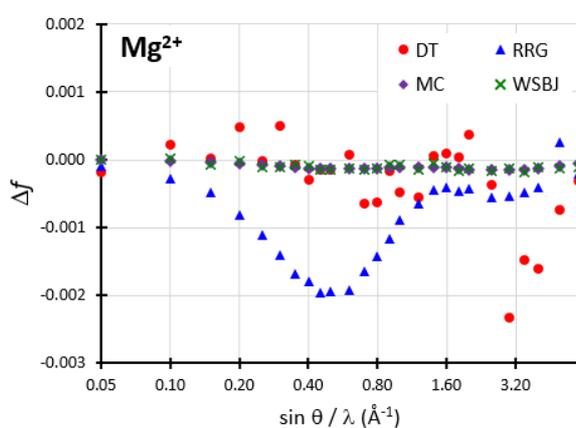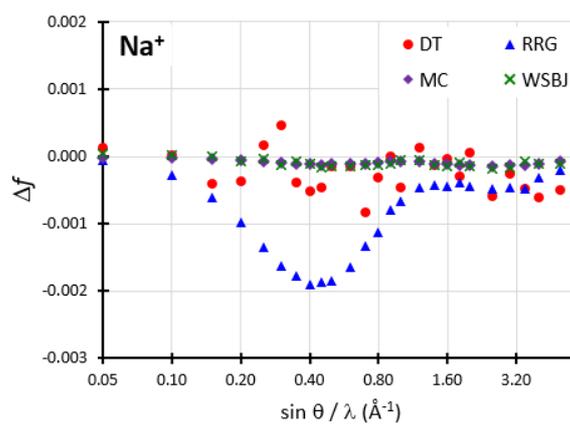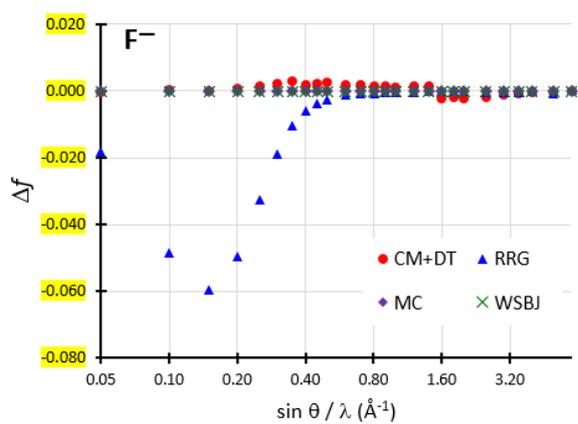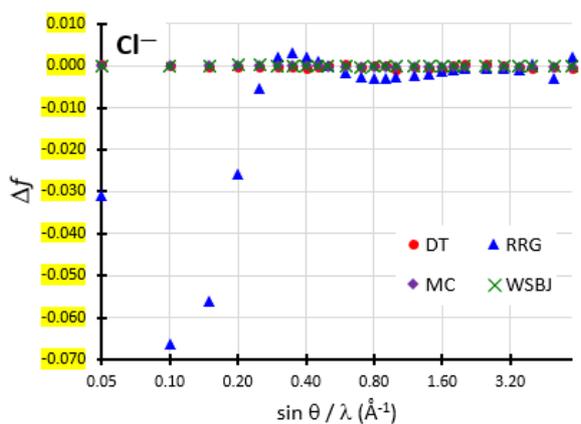
11) Cl⁻
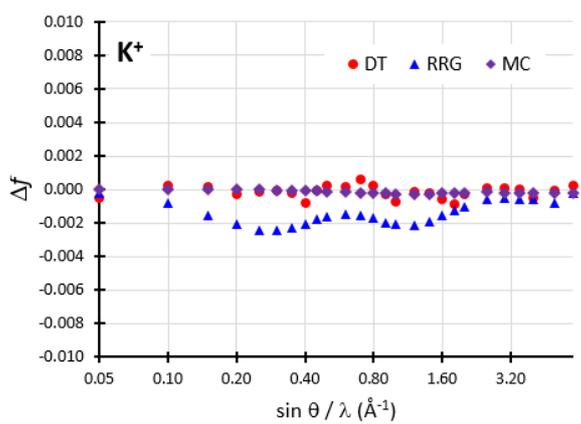
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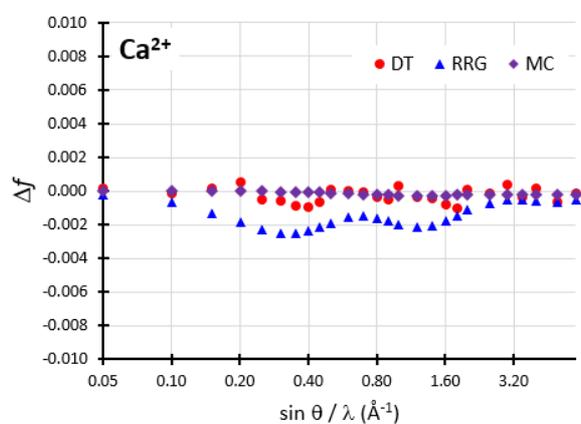
13) Ca²⁺
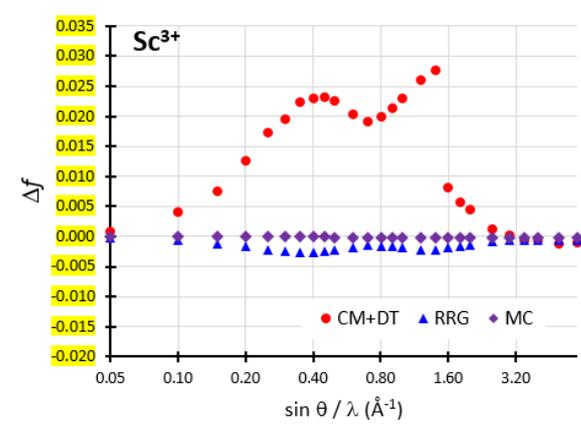
14) Sc³⁺
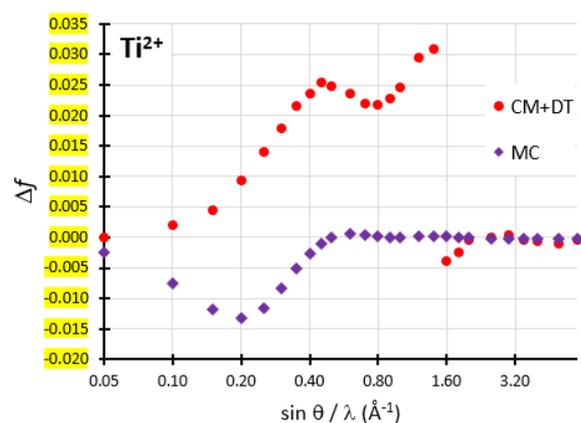
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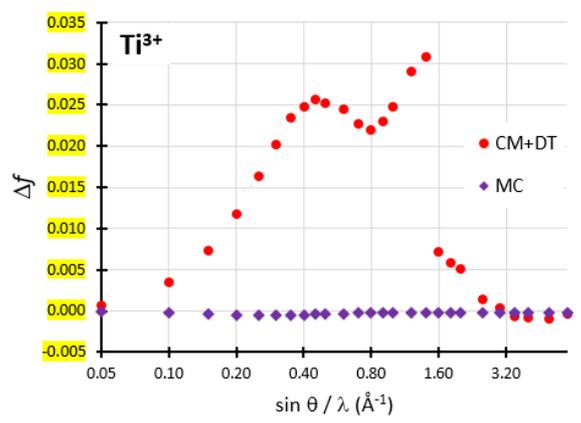
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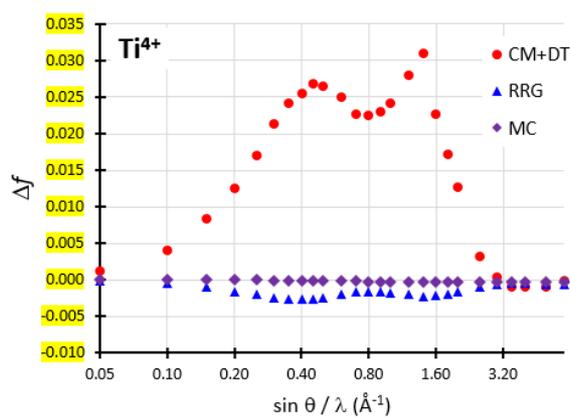
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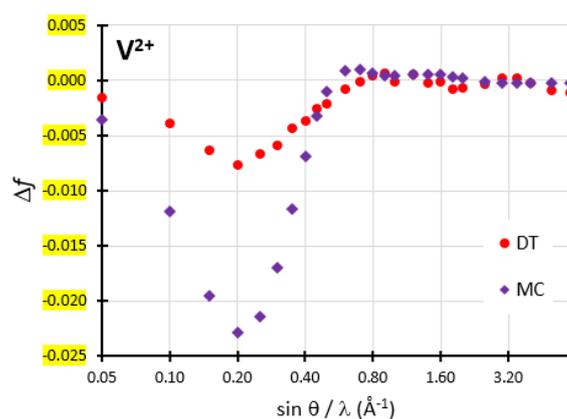
18) V²⁺
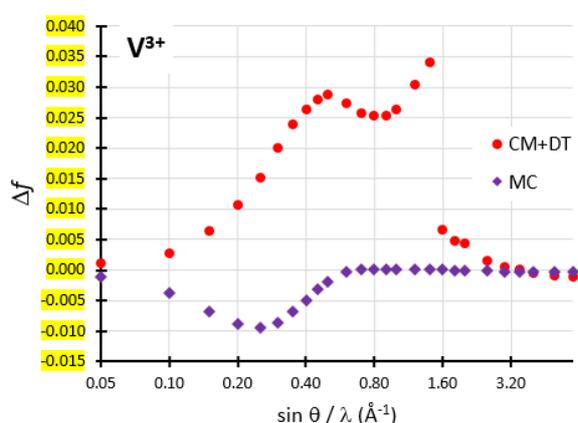
19) V³⁺
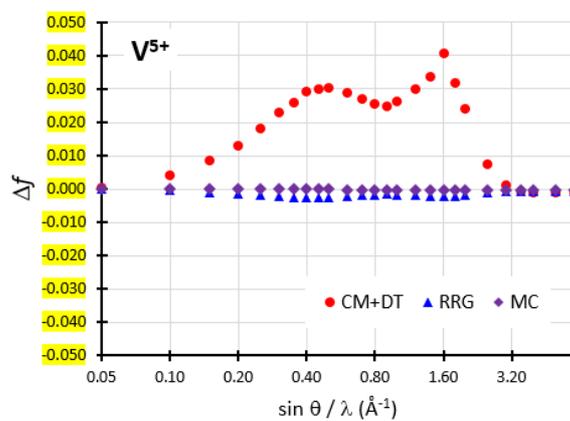
20) V⁵⁺
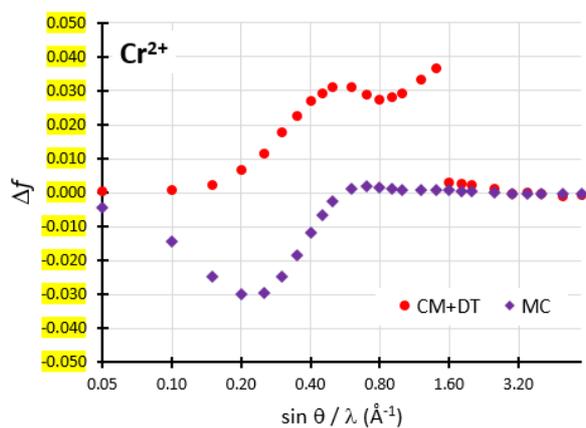
21) Cr²⁺
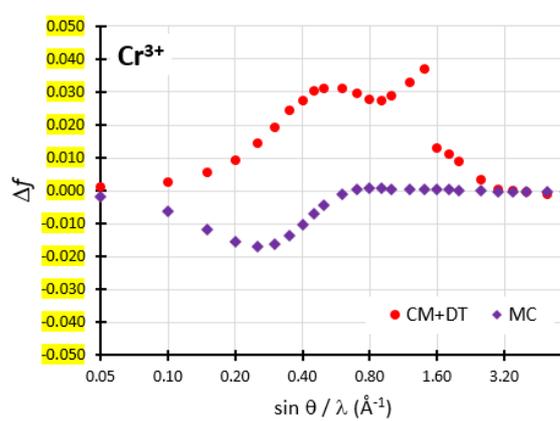
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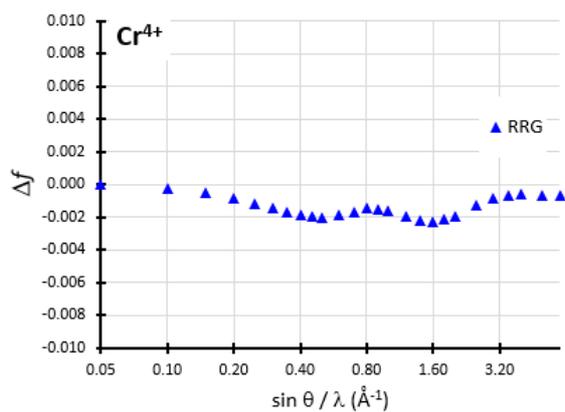
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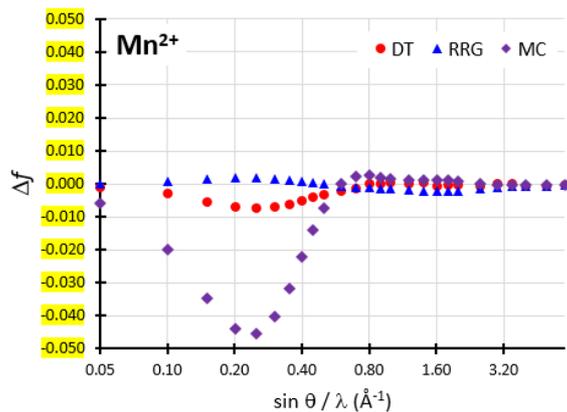
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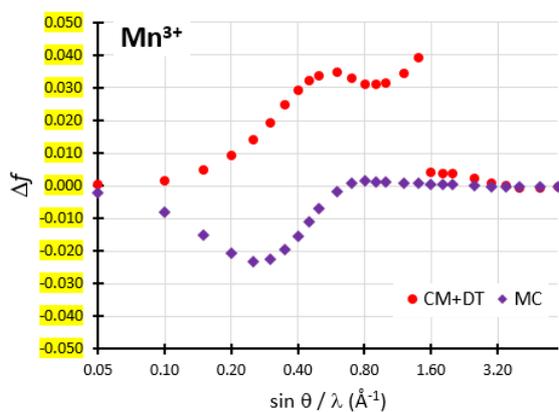
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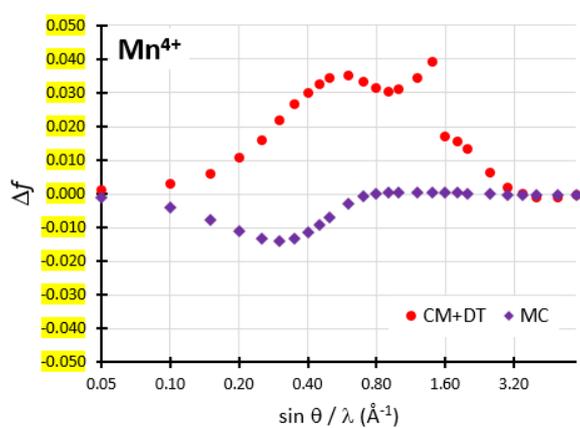
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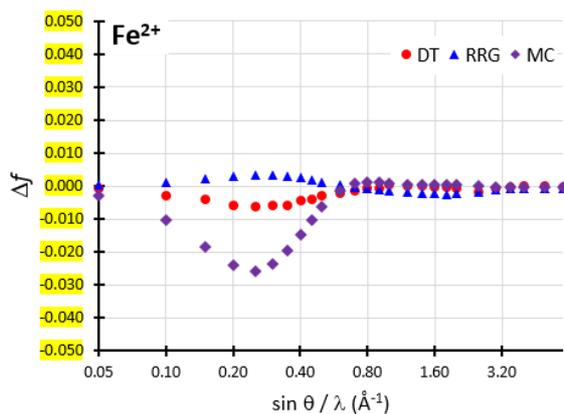
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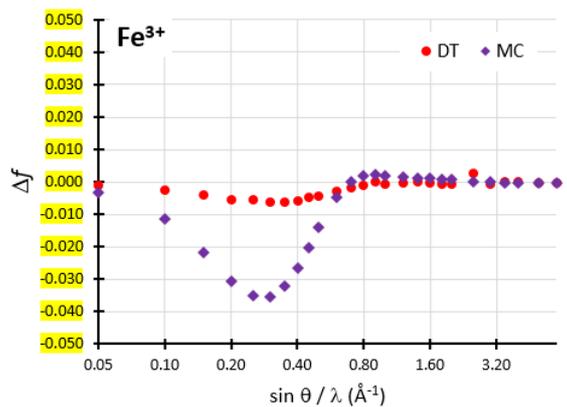
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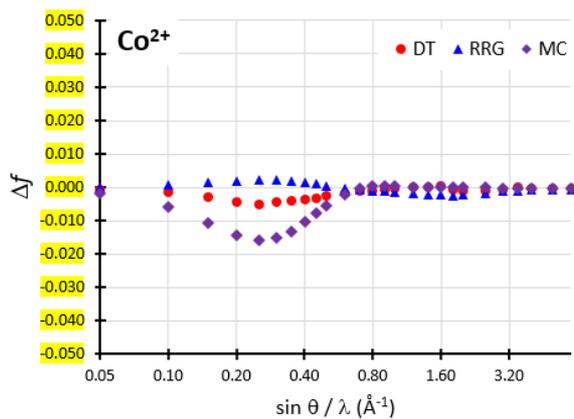
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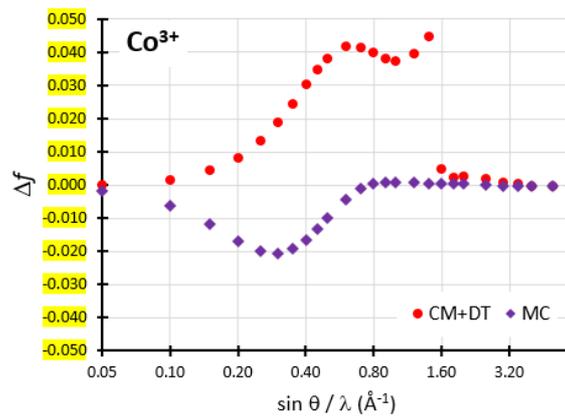
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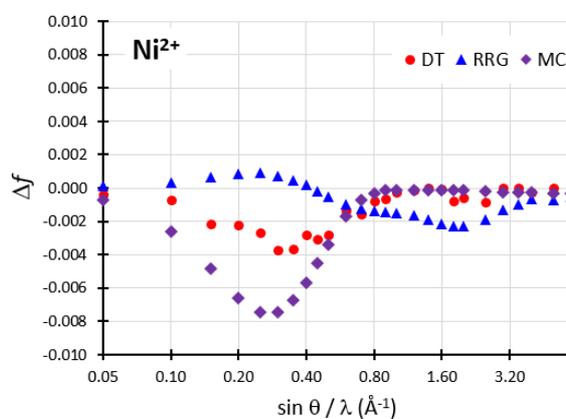
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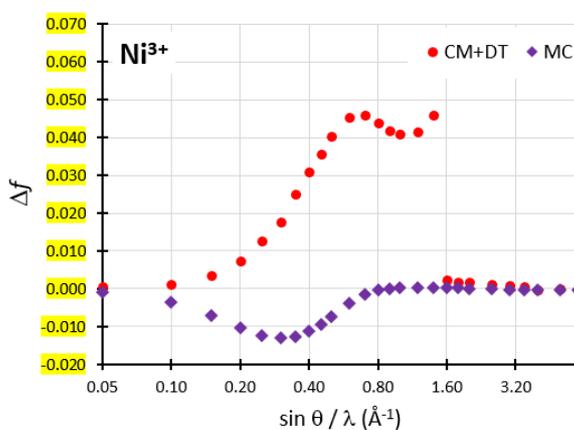
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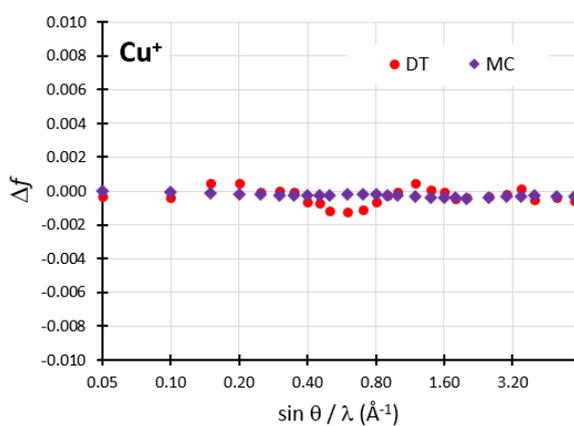
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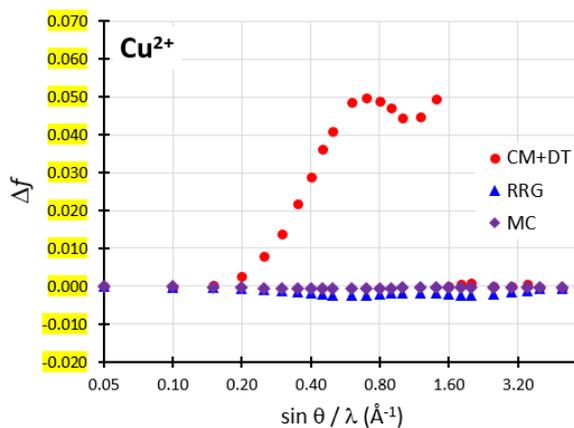
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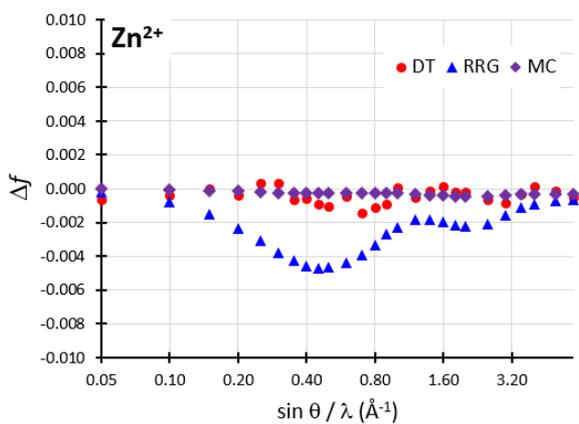
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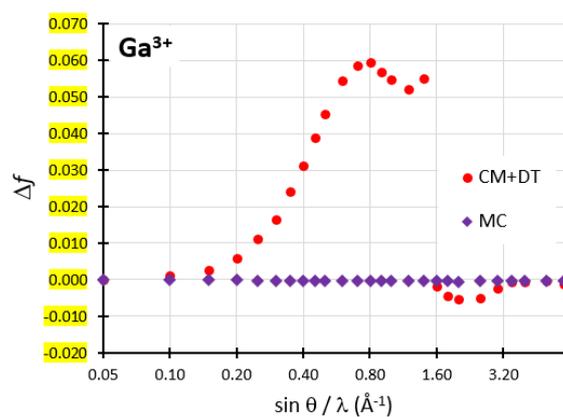
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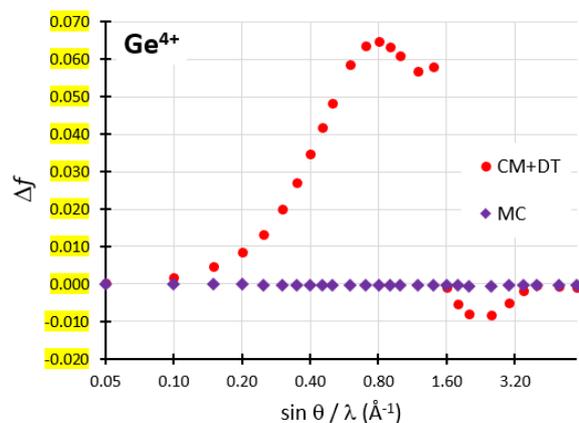
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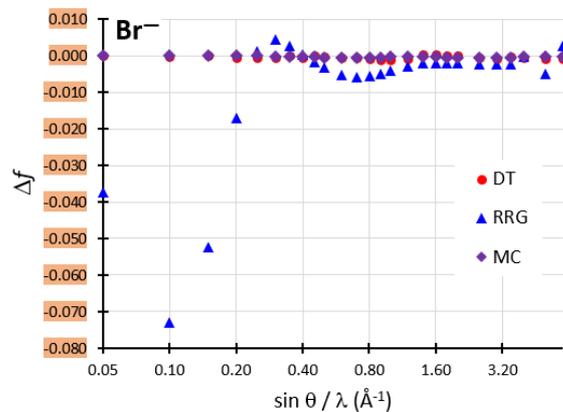
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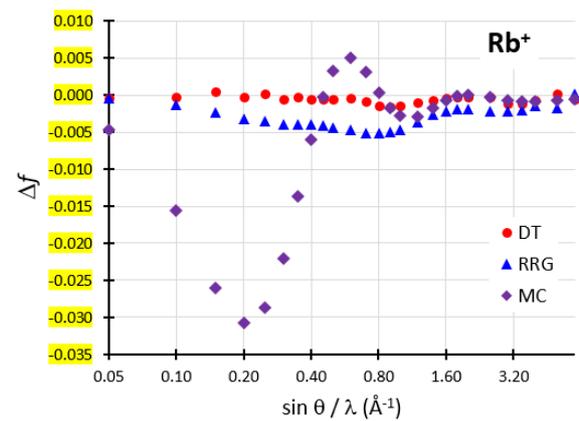
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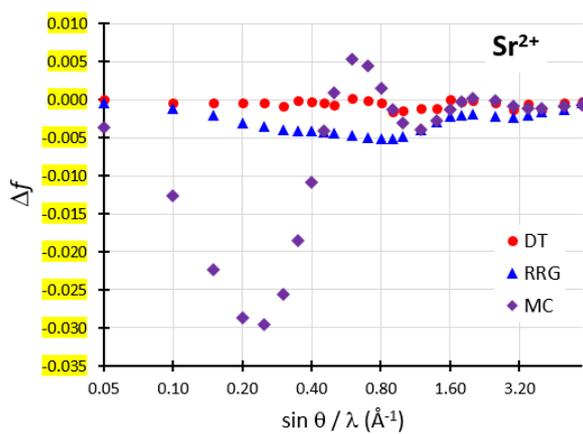
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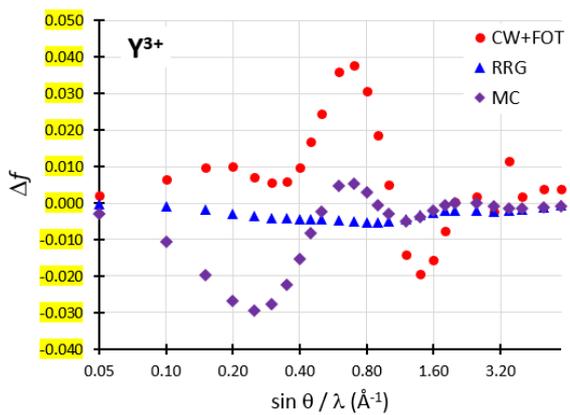
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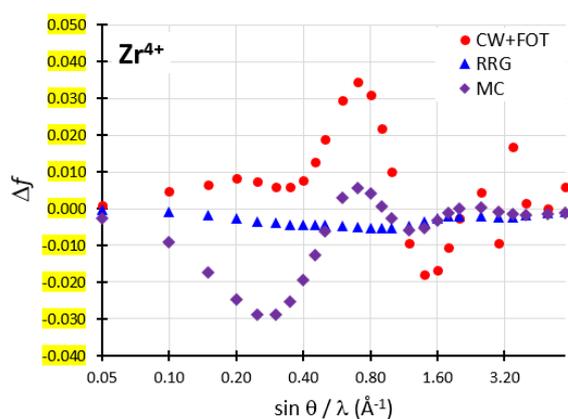
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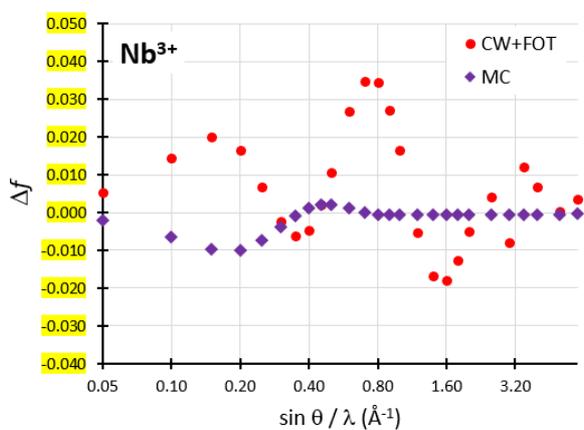
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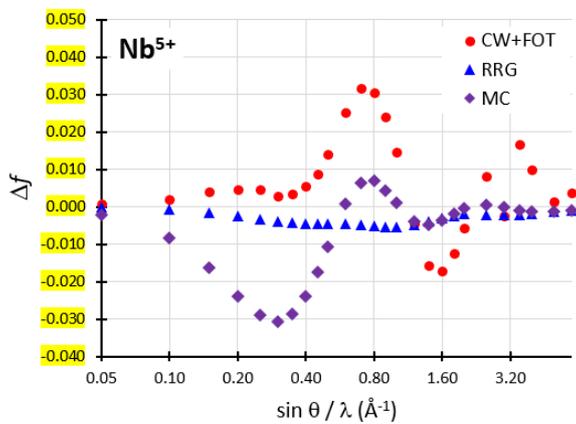
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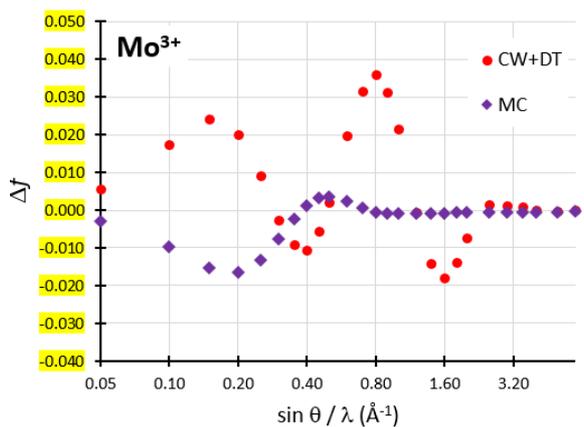
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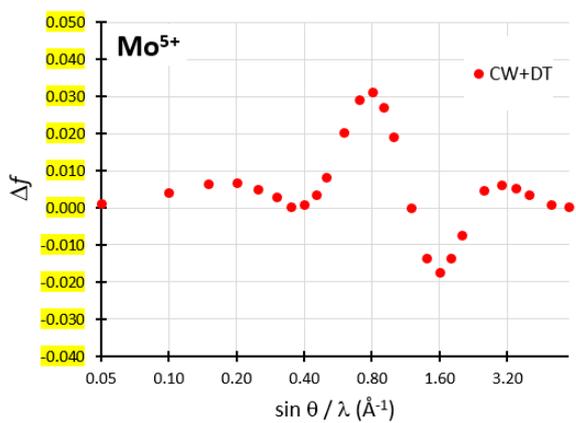
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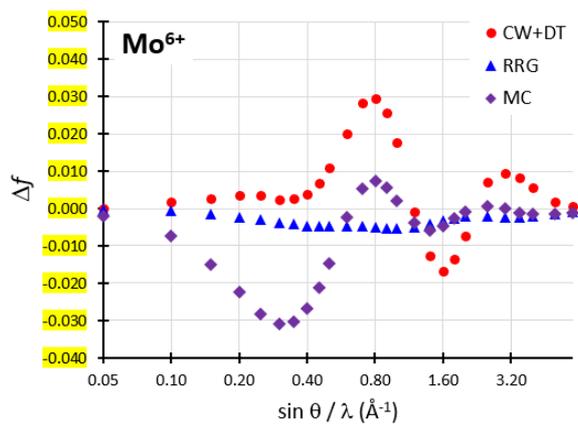
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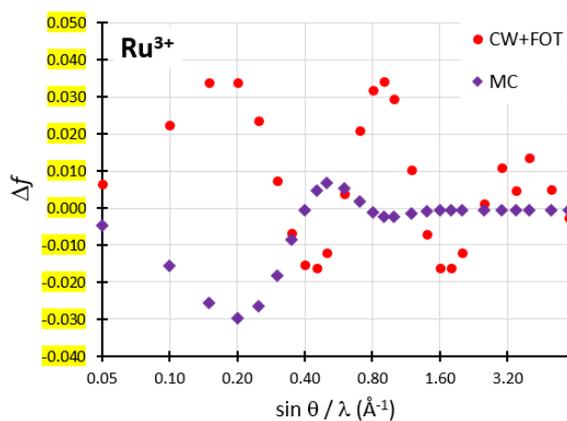
48) Ru^{3+}
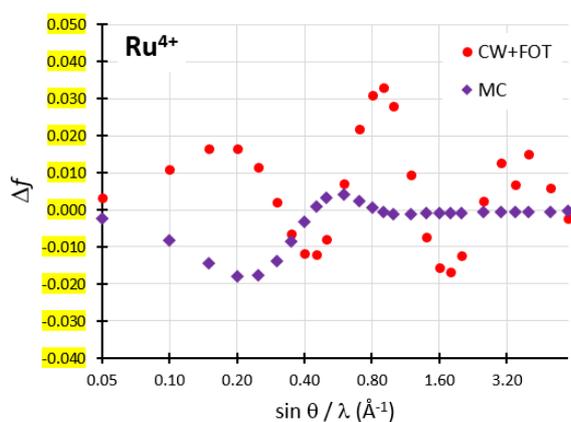
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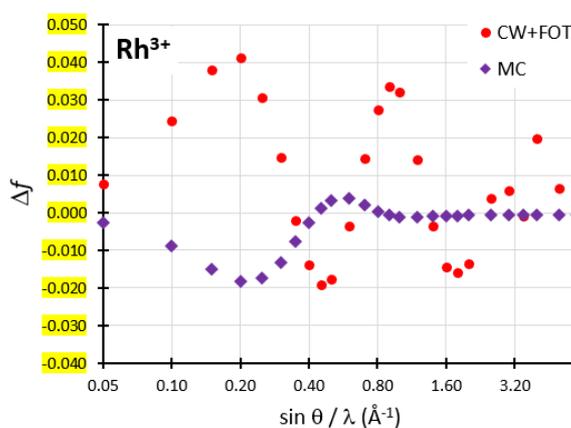
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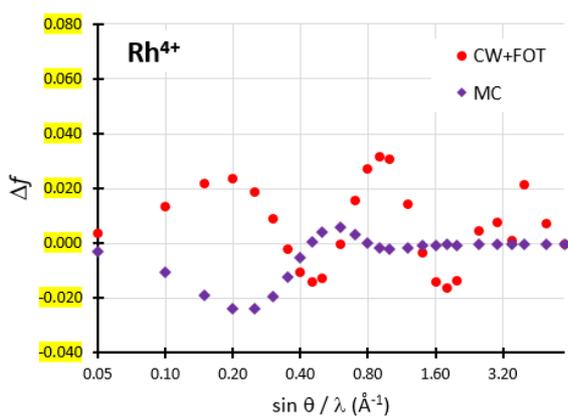
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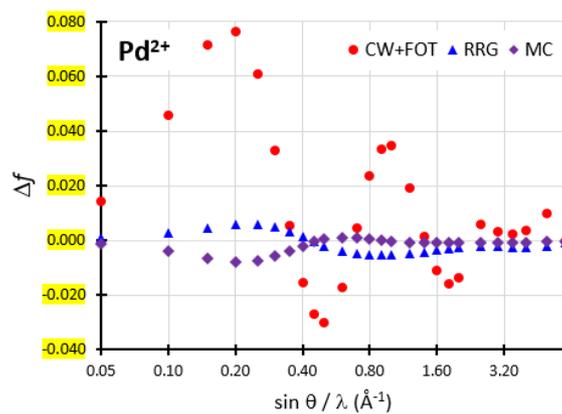
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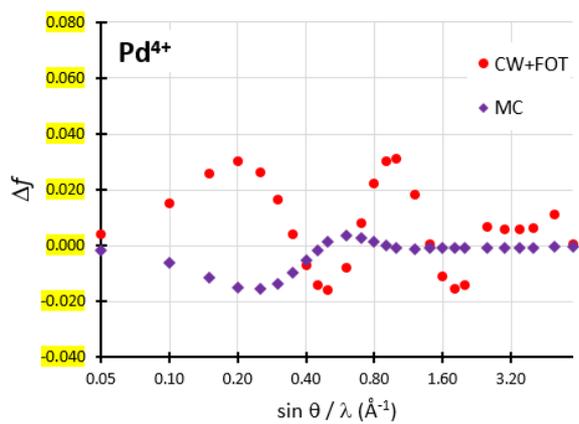
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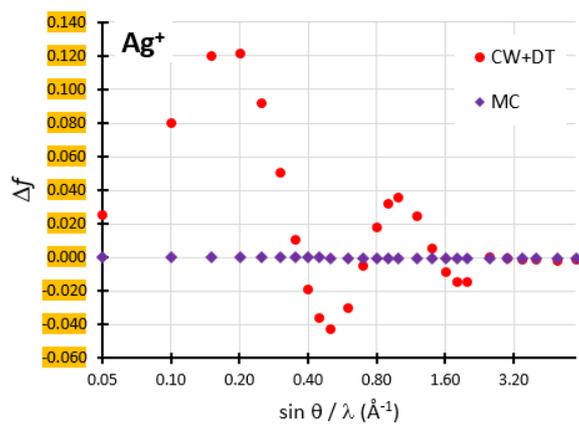
54) Ag^{+}
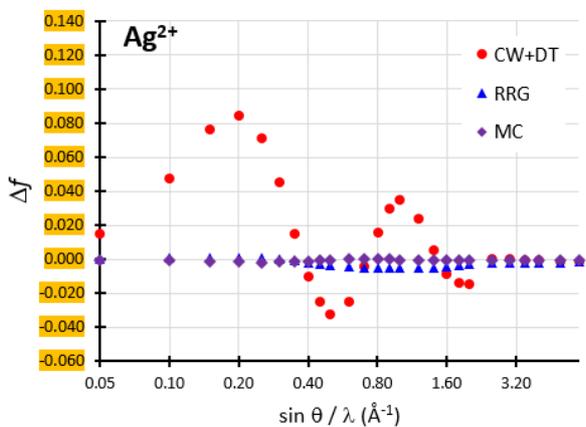
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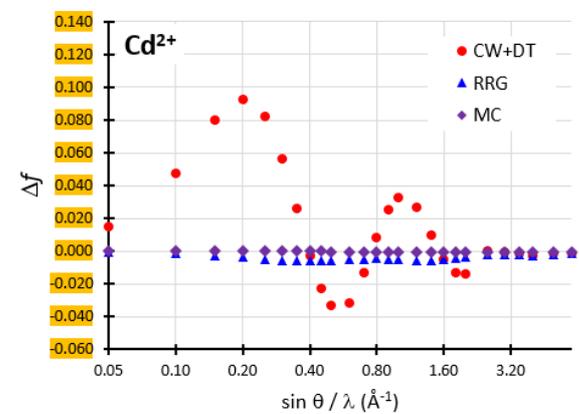
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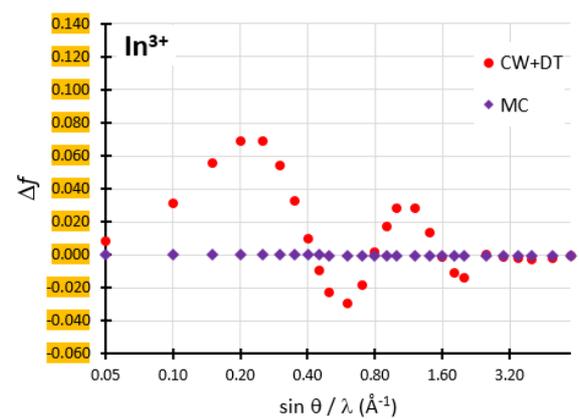
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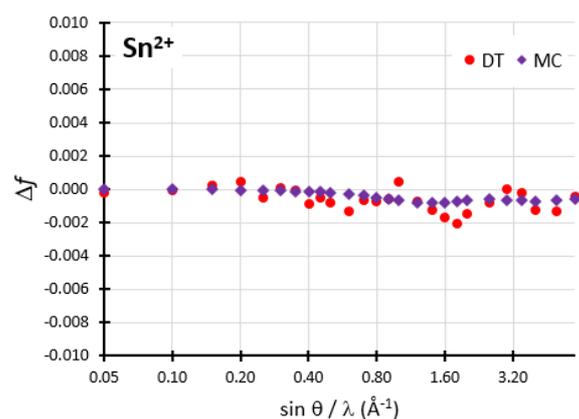
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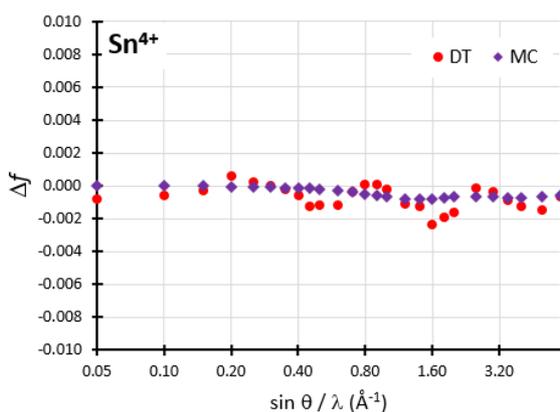
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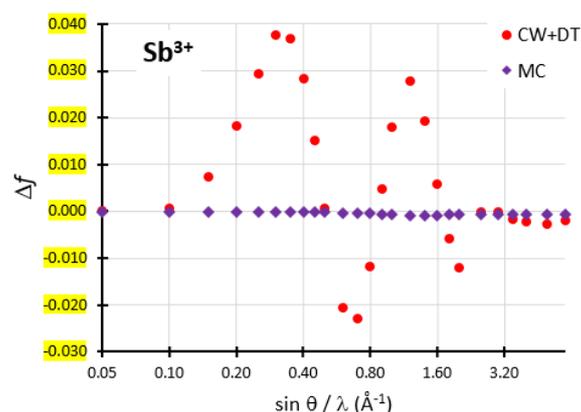
60) Sb³⁺
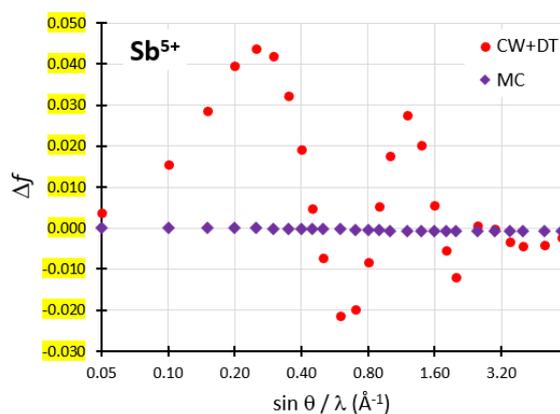
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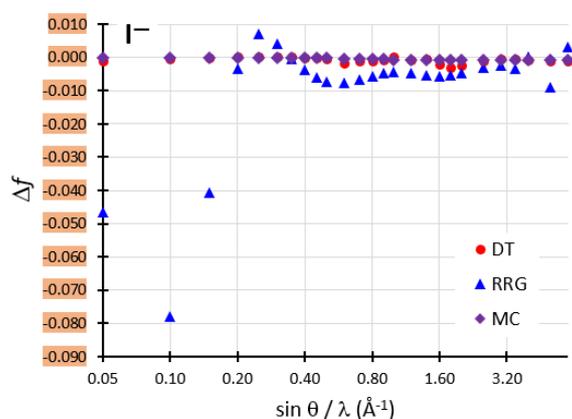
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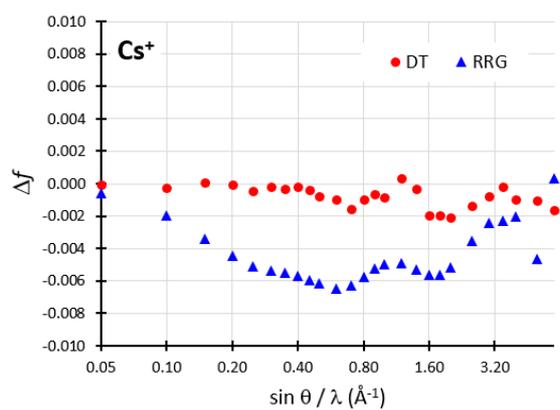
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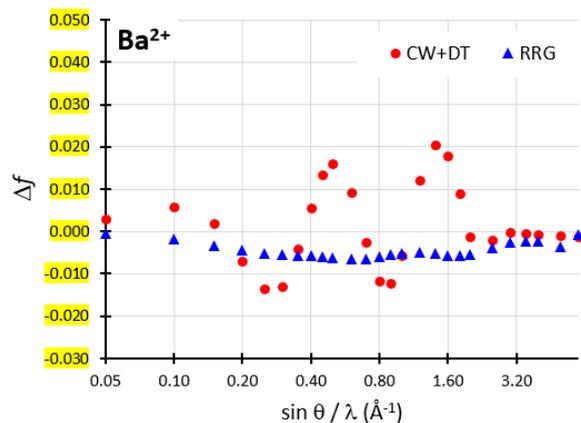
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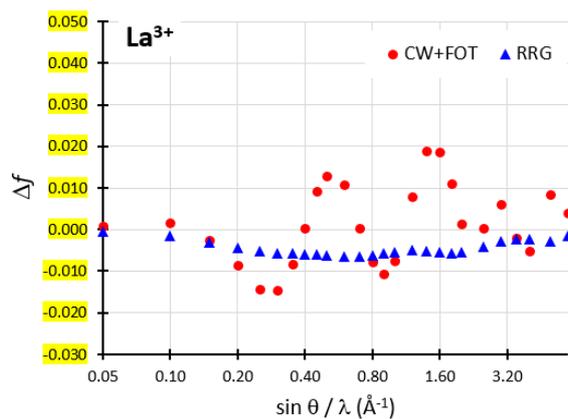
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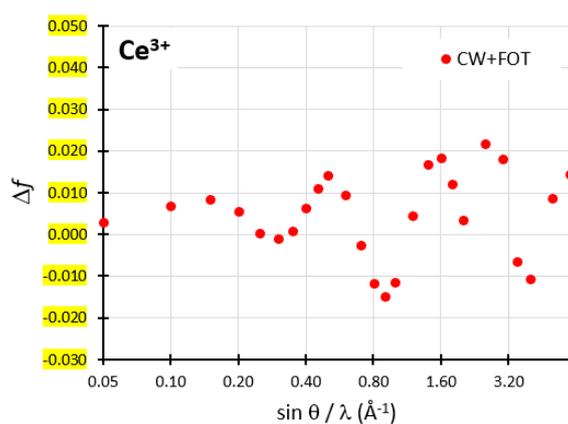
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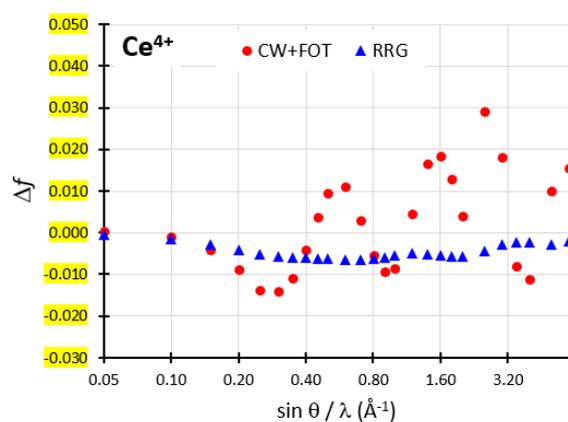
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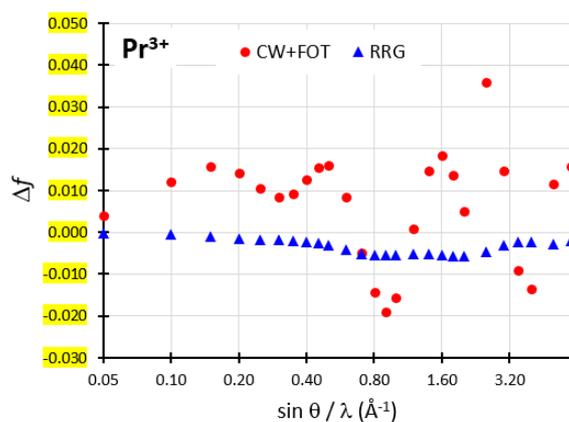
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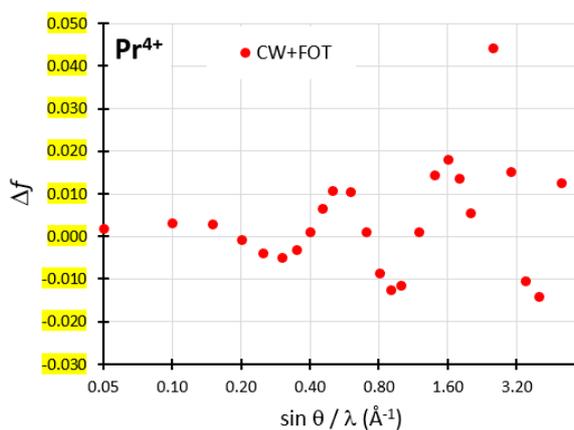
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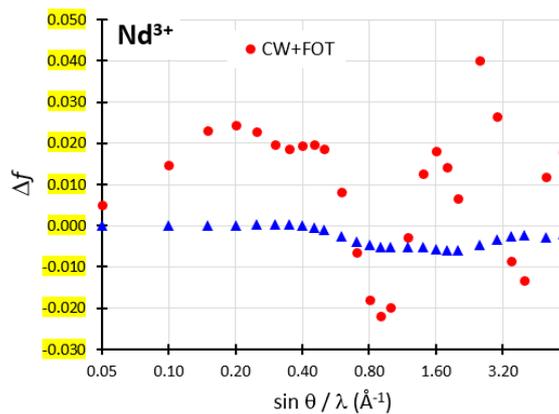
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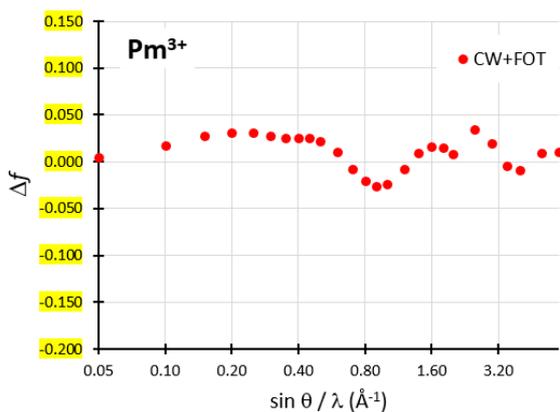
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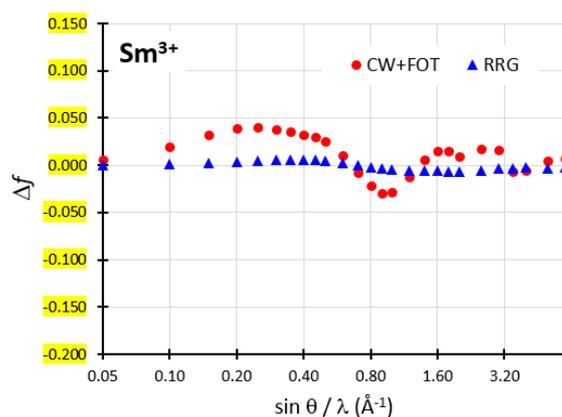
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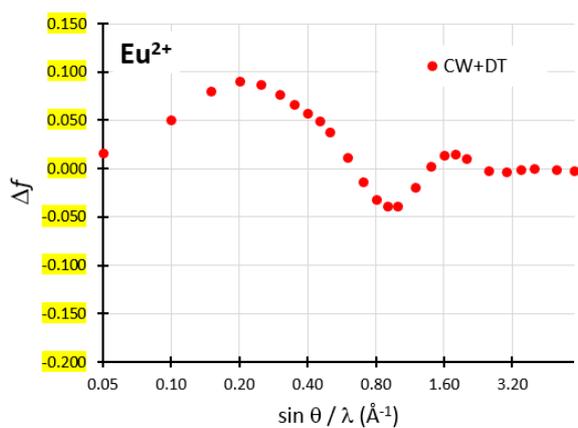
73) Eu²⁺
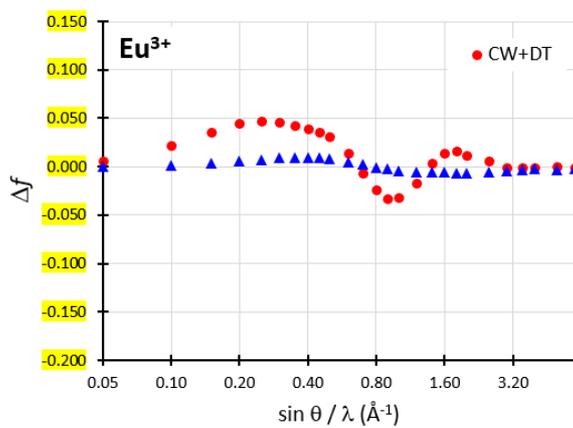
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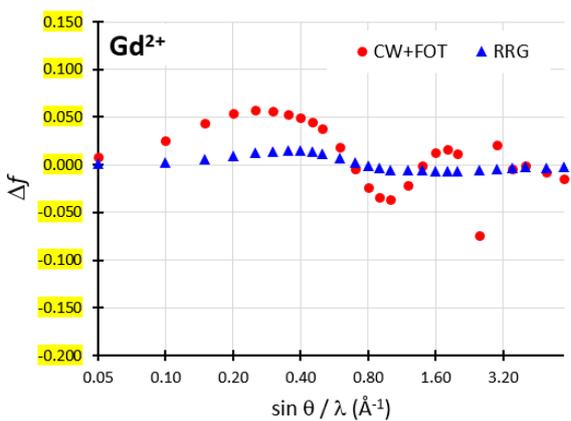
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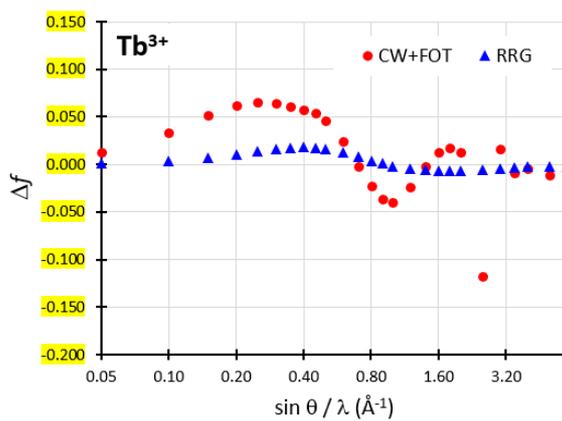
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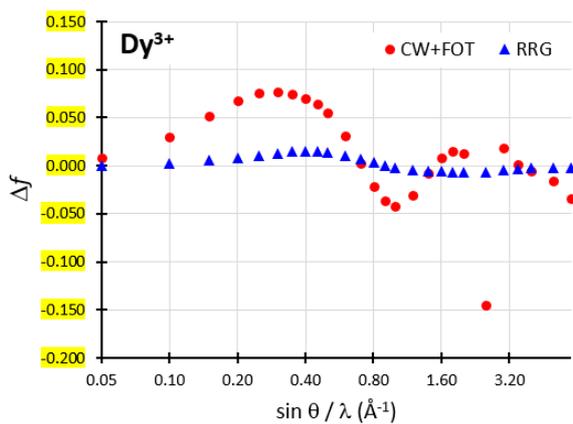
77) Dy³⁺
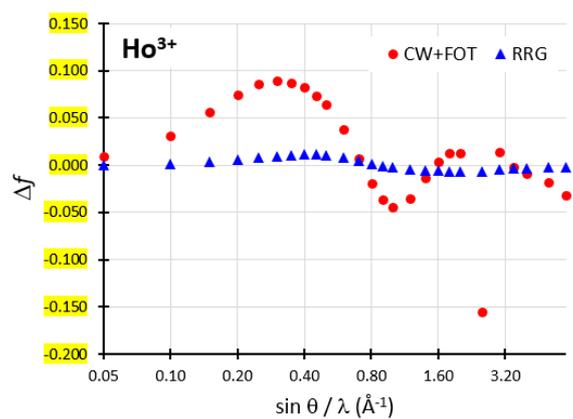
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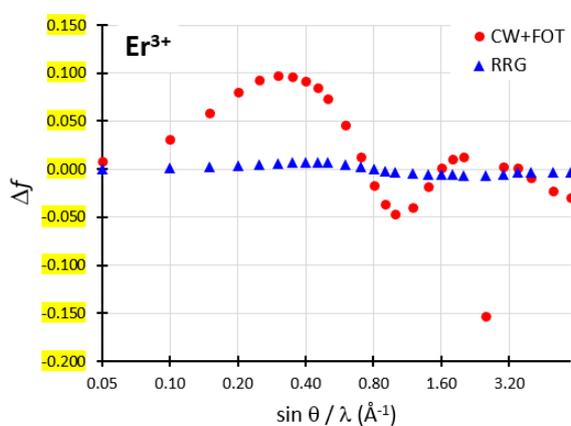
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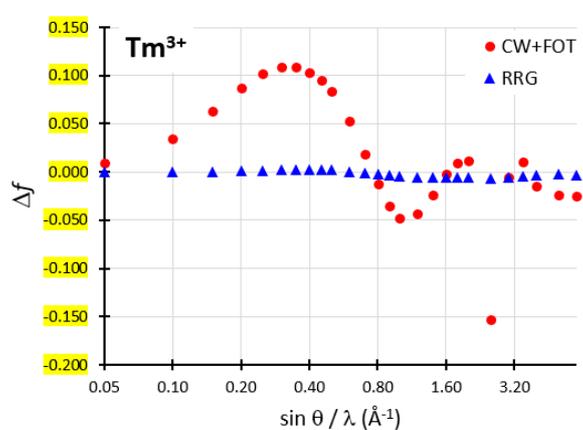
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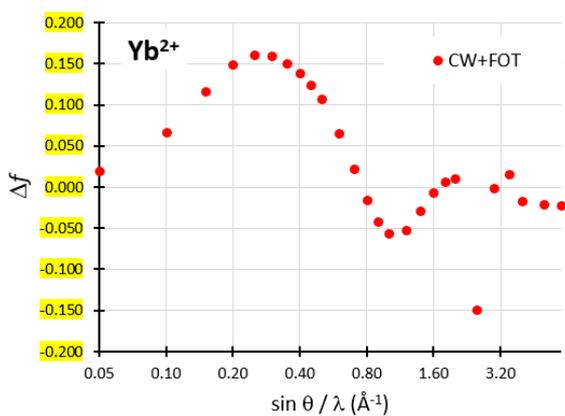
81) Yb²⁺
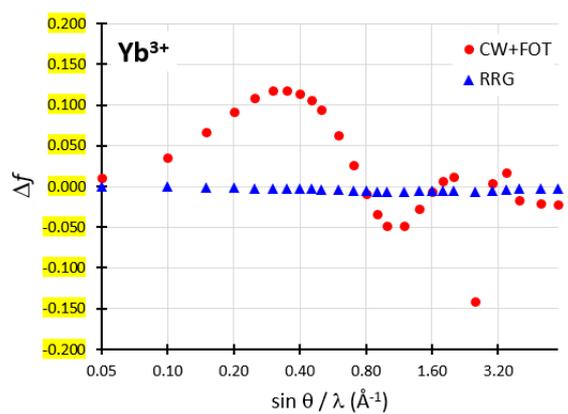
82) Yb³⁺
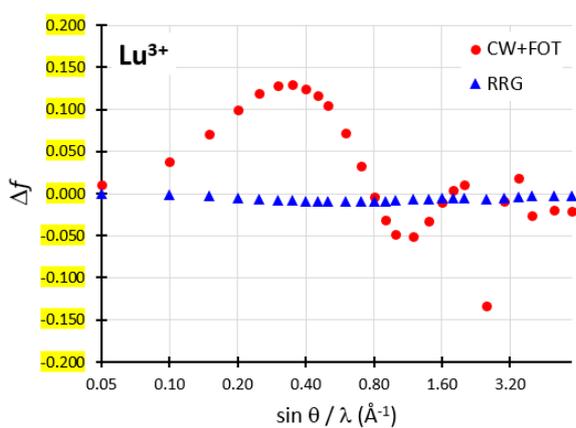
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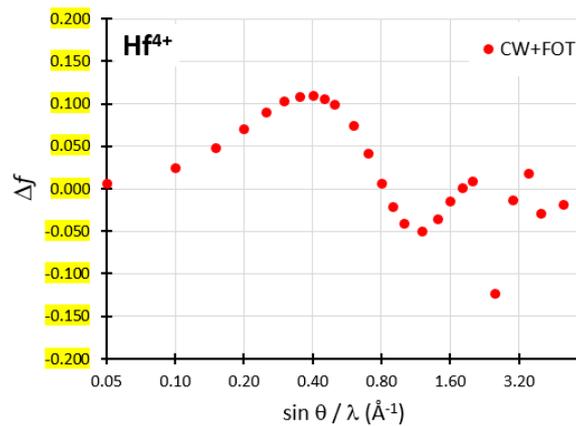
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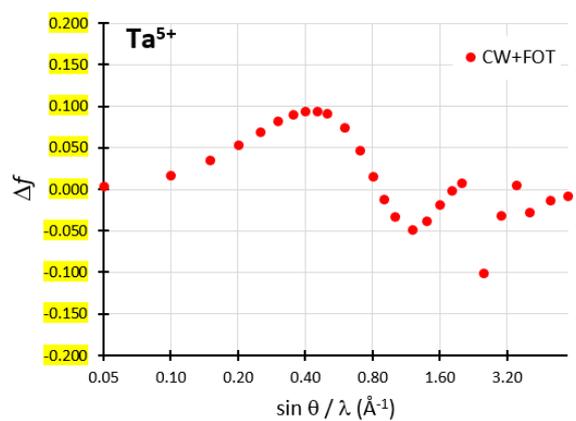
85) Ta⁵⁺
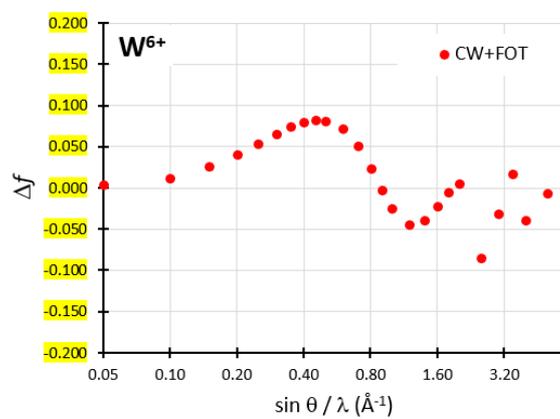
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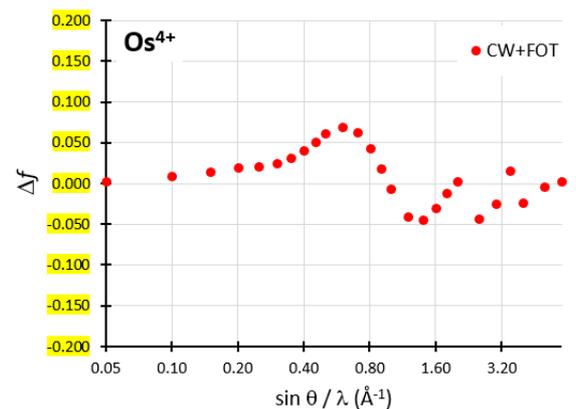
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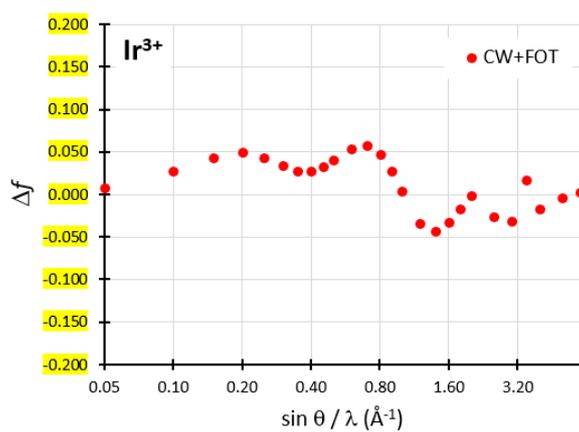
88) Ir³⁺
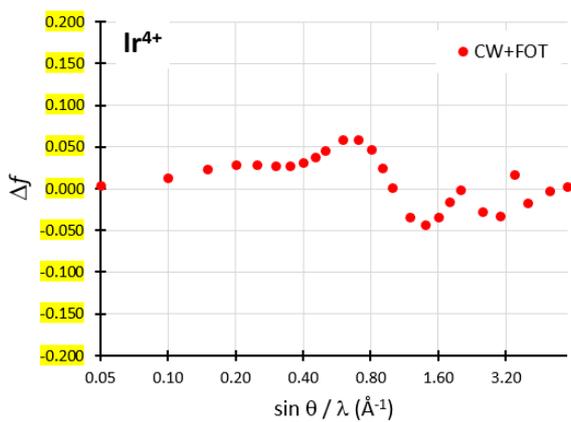
89) Ir^{4+}
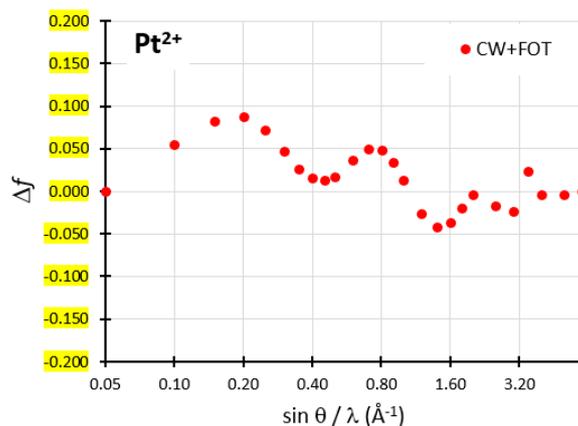
90) Pt^{2+}
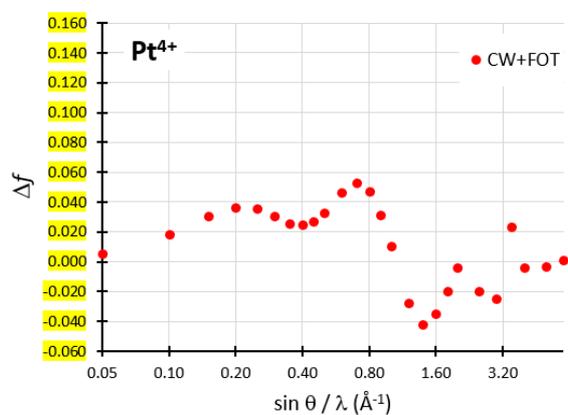
91) Pt^{4+}
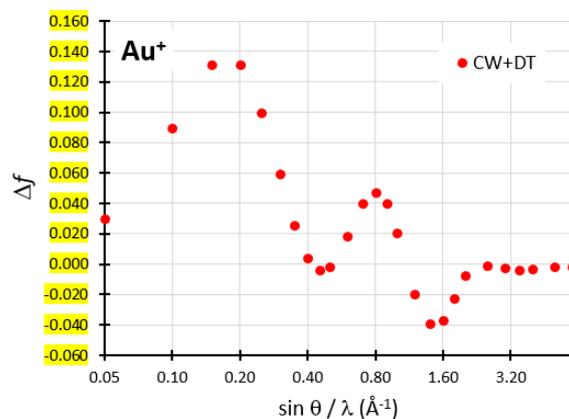
92) Au^{+}
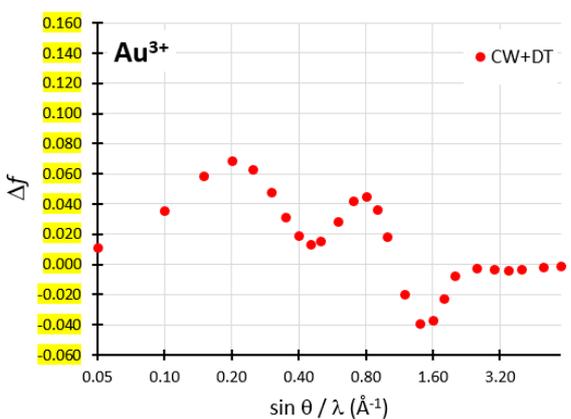
93) Au^{3+}
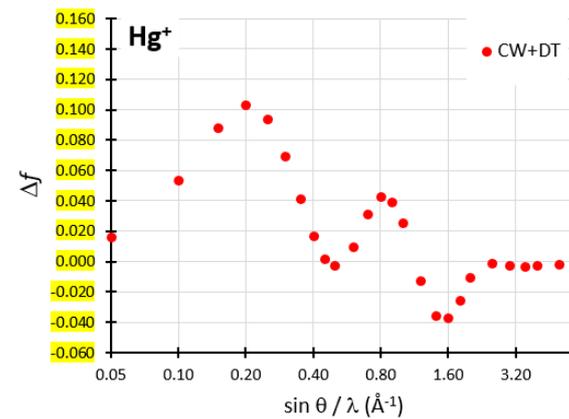
94) Hg^{+}
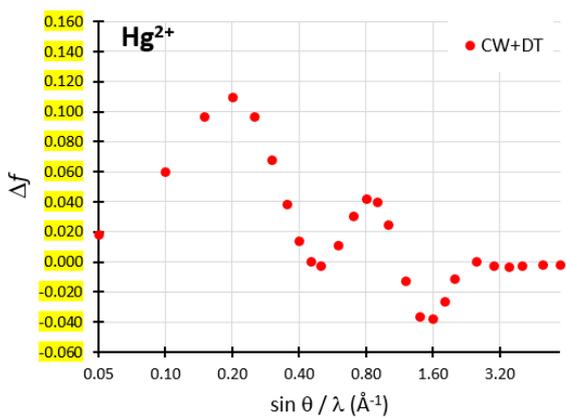
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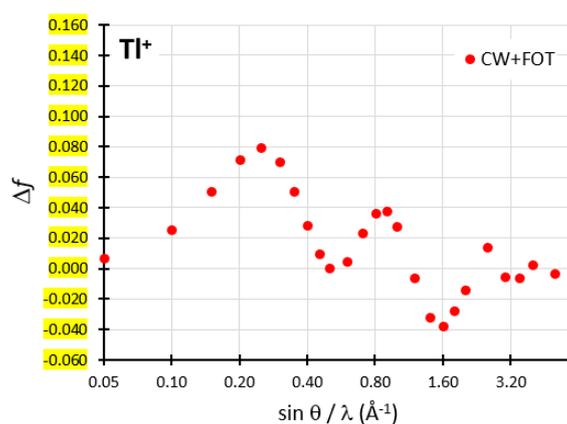
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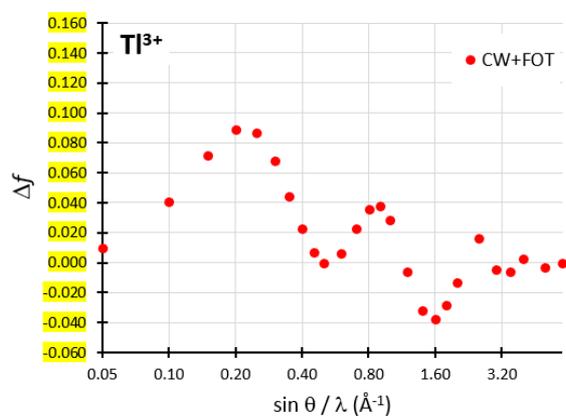
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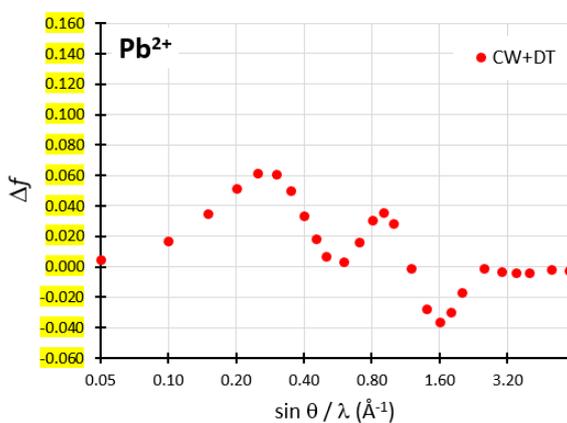
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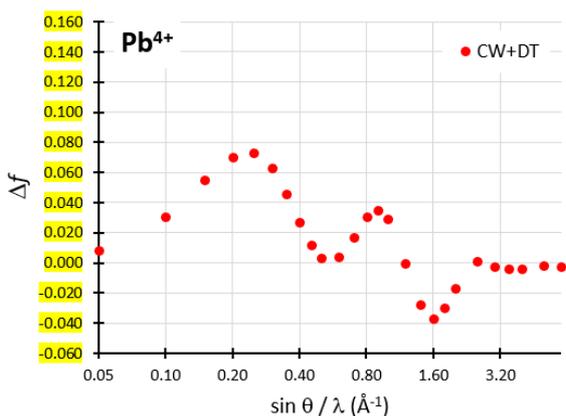
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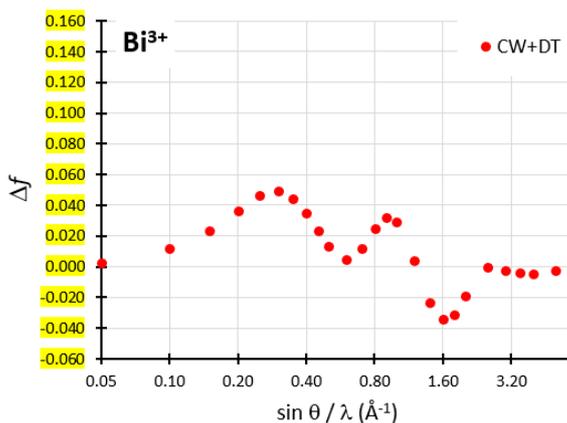
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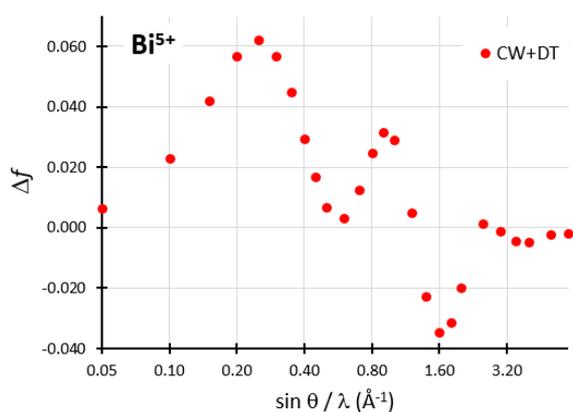
101) Bi^{5+}
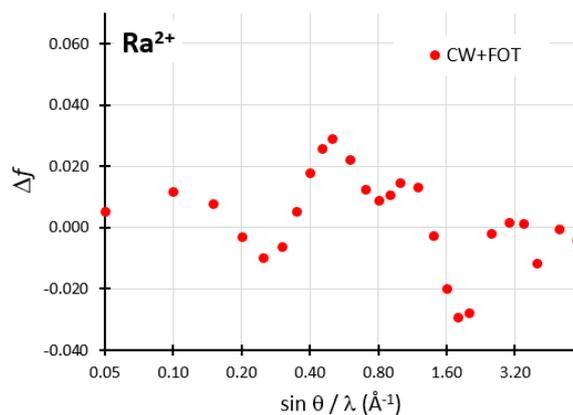
102) Ra^{2+}
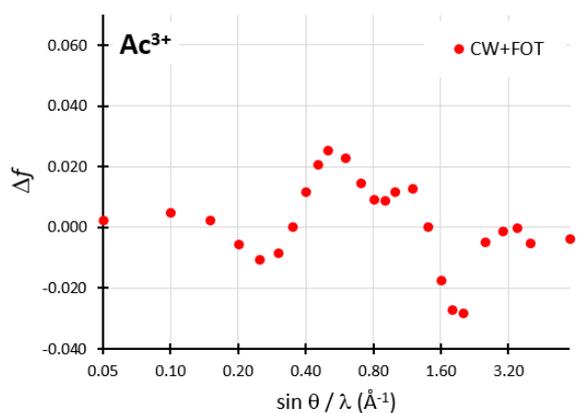
103) Ac^{3+}
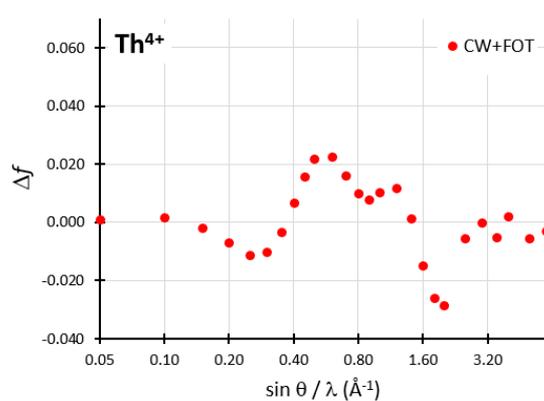
104) Th^{4+}
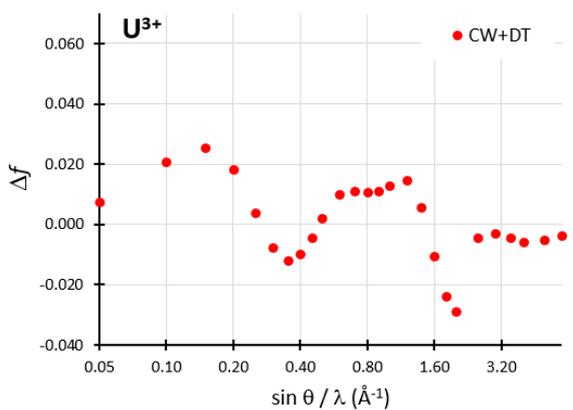
105) U^{3+}
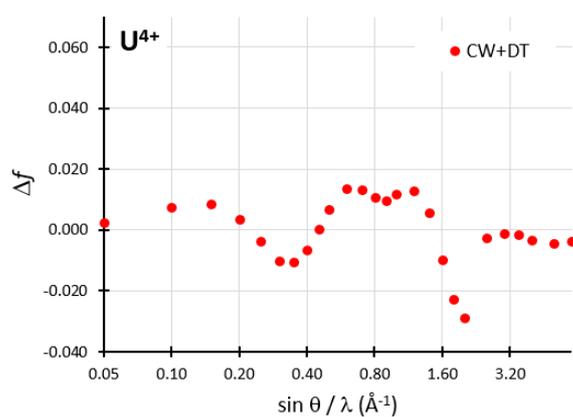
106) U^{4+}
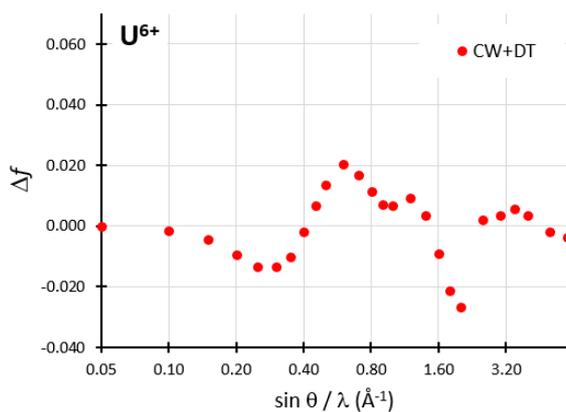
107) U^{6+}
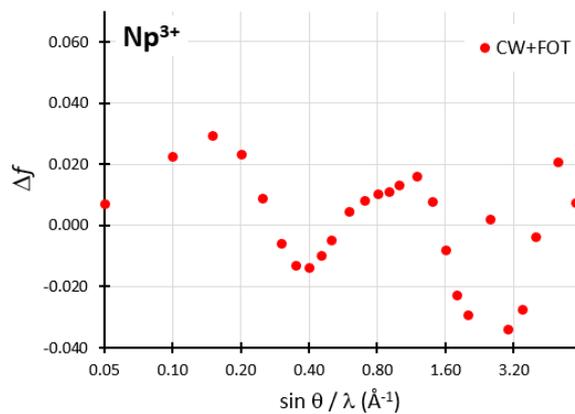
108) Np^{3+}
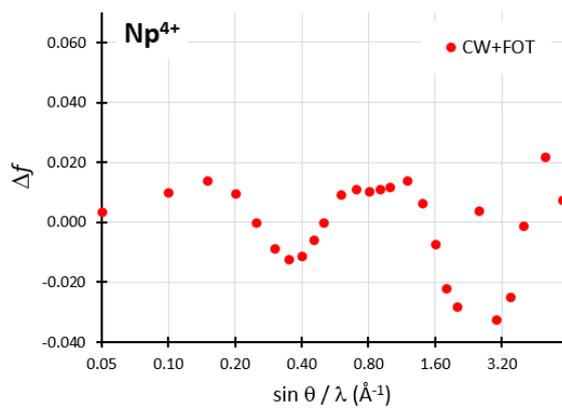
109) Np^{4+}
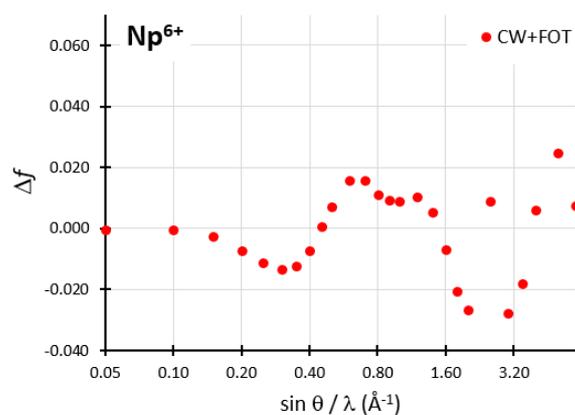
110) Np^{6+}
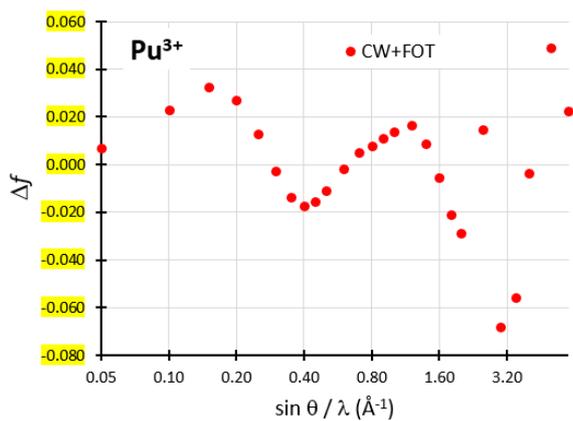
111) Pu^{3+}
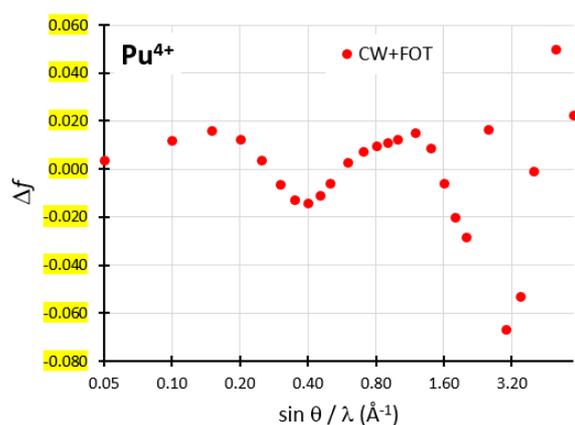
112) Pu^{4+}
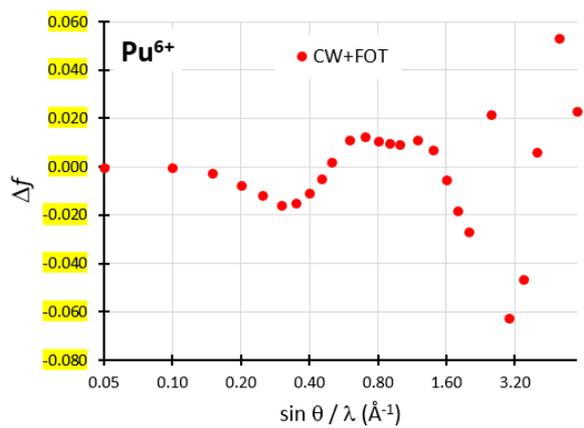
113) Pu⁶⁺

Figure S2. Selected ionization energies (eV) from this work, Wang et al. (1996), Macchi & Coppens (2001), Rodrigues et al. (2004), and Kramida et al. (2021): **(a)** first, **(b)** second, **(c)** third, **(d)** fourth, **(e)** fifth, **(f)** sixth, **(g)** seventh, and **(h)** eighth. Note that for the fourth and higher ionization energies, Kramida et al. (2021) data include the Rodrigues et al. (2004) values.

a)

b)

c)

d)

e)

f)

g)

h)