Chapter 1

De-novo design of metal binding moieties using machine learning

1.1 Background

1.2 Methods

1.2.1 Pseudo code

Result: Write here the result

foreach *whaoei* **do**

```
1 |  xxx;
```

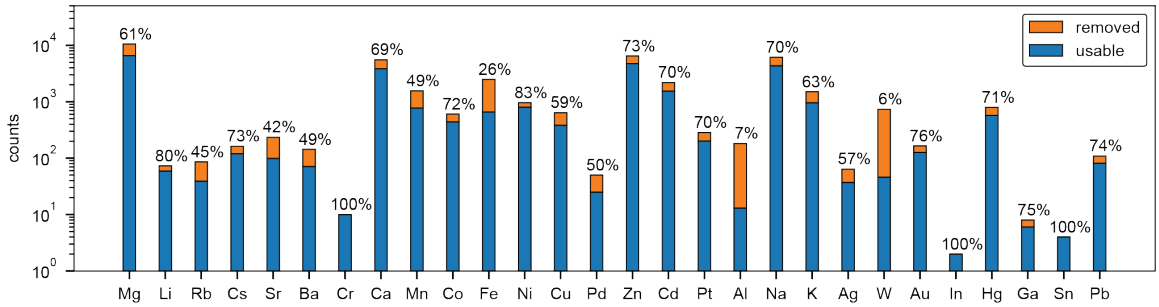
end

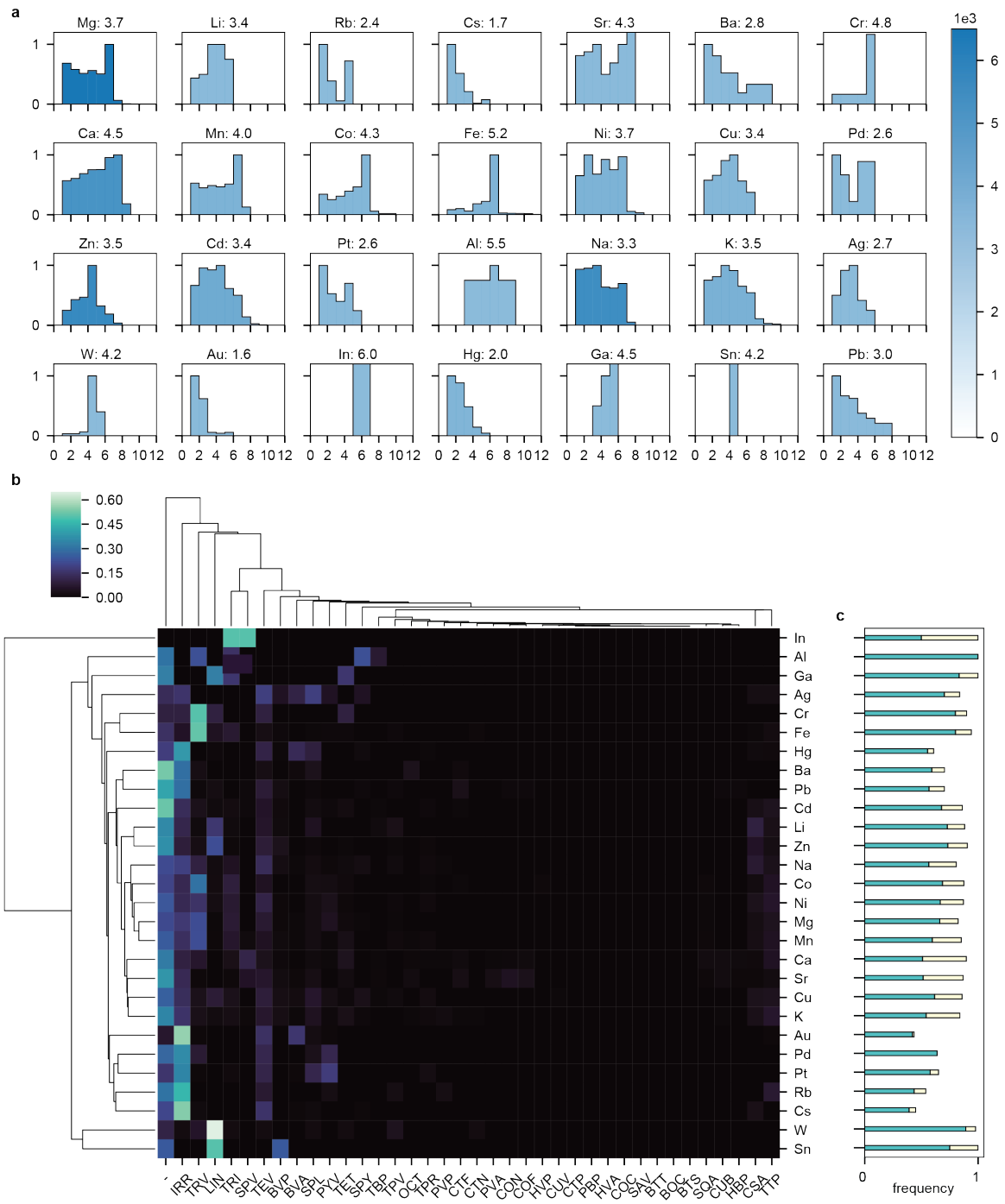
Algorithm 1: How to write algorithms

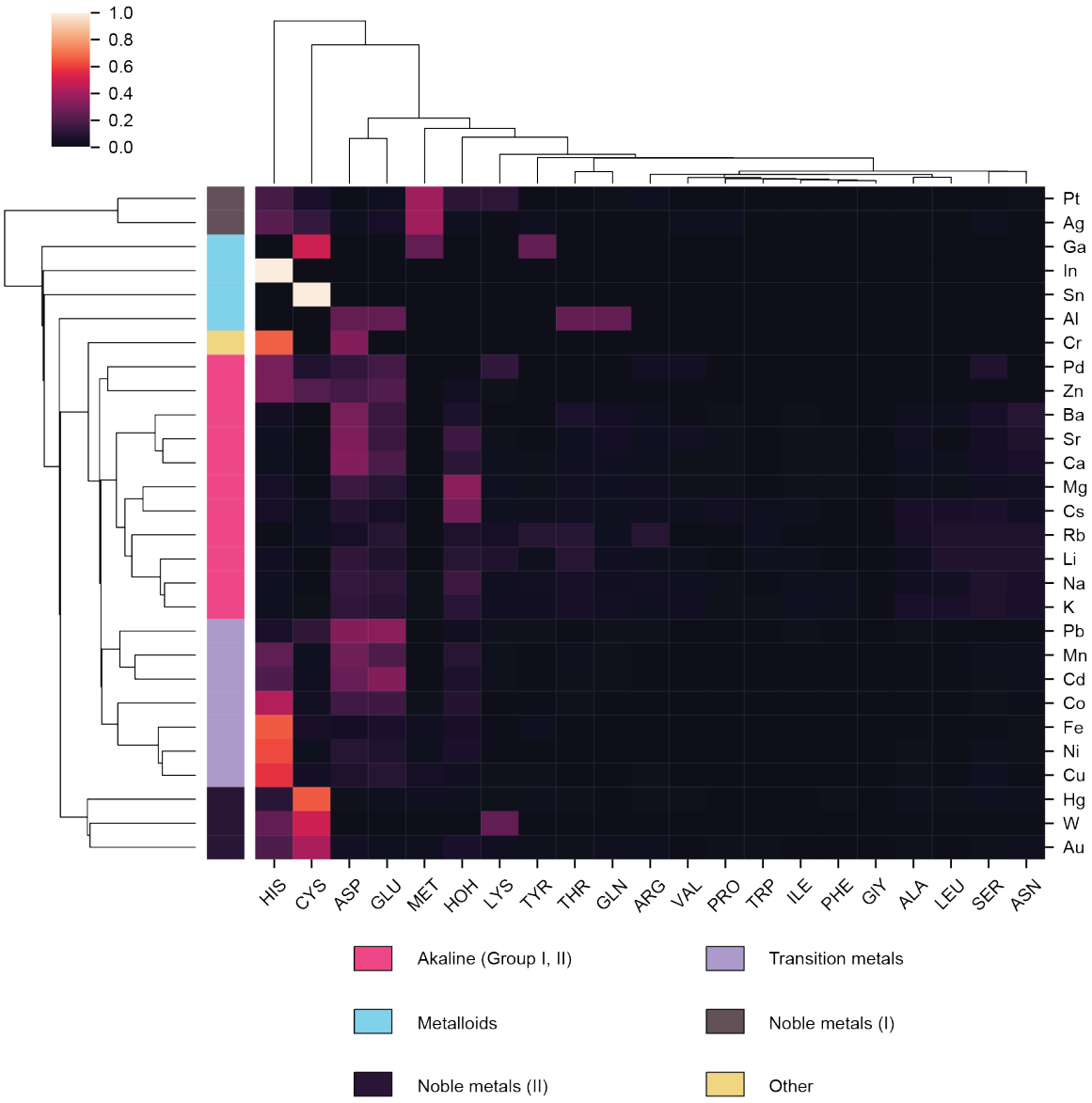
no.	val	abbrv	full geometry name	instances	percent
1	0	-	-	4086	15%
2	0	IRR	irregular	7530	28%
3	2	TRV	trigonal plane with a vacancy	2209	8%
4	2	LIN	linear	230	1%
5	3	TRI	trigonal plane	214	1%
6	3	SPV	square plane with a vacancy	634	2%
7	3	TEV	tetrahedron with a vacancy	1047	4%
8	4	BVP	trigonal bipyramid with a vacancy (equatorial)	234	1%
9	4	BVA	trigonal bipyramid with a vacancy (axial)	505	2%
10	4	SPL	square plane	537	2%
11	4	PYV	square pyramid with a vacancy (equatorial)	1124	4%
12	4	TET	tetrahedron	1405	5%
13	5	SPY	square pyramid	1247	5%
14	5	TBP	trigonal bipyramid	202	1%
15	5	TPV	trigonal prism with a vacancy	87	0%
16	6	OCT	octahedron	3219	12%
17	6	TPR	trigonal prism	49	0%
18	6	PVP	pentagonal bipyramid with a vacancy (equatorial)	491	2%
19	6	CTF	trigonal prism, square-face monocapped with a vacancy (capped face)	40	0%
20	6	CTN	trigonal prism, square-face monocapped with a vacancy (non-capped edge)	95	0%
21	6	PVA	pentagonal bipyramid with a vacancy (axial)	129	0%
22	6	CON	octahedron face monocapped with a vacancy (non-capped face)	77	0%
23	6	COF	octahedron face monocapped with a vacancy (capped face)	71	0%
24	7	HVP	hexagonal bipyramid with a vacancy (equatorial)	49	0%
25	7	CUV	cube with a vacancy	4	0%
26	7	CTP	trigonal prism square-face monocapped	99	0%
27	7	PBP	pentagonal bipyramid	544	2%
28	7	HVA	hexagonal bipyramid with a vacancy (axial)	2	0%
29	7	COC	octahedron face monocapped	148	1%
30	7	SAV	square antiprism with a vacancy	83	0%
31	8	BTT	trigonal prism triangular-face bicapped	0	0%
32	8	BOC	octahedron trans-bicapped	0	0%
33	8	BTS	trigonal prism square-face bicapped	56	0%
34	8	SQA	square antiprism	79	0%
35	8	CUB	cube	3	0%
36	8	HBP	hexagonal bipyramid	5	0%
37	9	CSA	square antiprism square-face monocapped	0	0%
38	9	TTP	trigonal prism square-face tricapped	0	0%

1.3 Results

1.3.1 First Glance




a
Mg: 3.7
Li: 3.4
Rb: 2.4
Cs: 1.7
Sr: 4.3
Ba: 2.8
Cr: 4.8
Ca: 4.5
Mn: 4.0
Co: 4.3
Fe: 5.2
Ni: 3.7
Cu: 3.4
Pd: 2.6
Zn: 3.5
Cd: 3.4
Pt: 2.6
Al: 5.5
Na: 3.3
K: 3.5
Ag: 2.7
W: 4.2
Au: 1.6
In: 6.0
Hg: 2.0
Ga: 4.5
Sn: 4.2
Pb: 3.0
1e3
b
0.60
0.45
0.30
0.15
0.00
In
Al
Ga
Ag
Cr
Fe
Hg
Ba
Pb
Cd
Li
Zn
Na
Co
Ni
Mg
Mn
Ca
Sr
Cu
K
Au
Pd
Pt
Rb
Cs
W
Sn
IRR
TRV
LIN
TRI
SPV
TEV
BVP
BVA
SPL
PYV
TET
SPY
TBP
TPV
OCT
TPR
PVP
CTF
CTN
PVA
CON
COF
HVP
CUV
CTP
PBP
HVA
COC
SAV
BTT
BOC
BTS
SQA
CUB
HBP
CSA
TTP
c
frequency


1.0
0.8
0.6
0.4
0.2
0.0
Pt
Ag
Ga
In
Sn
Al
Cr
Pd
Zn
Ba
Sr
Ca
Mg
Cs
Rb
Li
Na
K
Pb
Mn
Cd
Co
Fe
Ni
Cu
Hg
W
Au
HIS
CYS
ASP
GLU
MET
HOH
LYS
TYR
THR
GLN
ARG
VAL
PRO
TRP
ILE
PHE
GlY
ALA
LEU
SER
ASN
Akaline (Group I, II)
Transition metals
Metalloids
Noble metals (I)
Noble metals (II)
Other

	HIS	CYS	ASP	GLU	MET	HOH	LYS	TYR	THR	GLN	ARG	VAL	PRO	TRP	ILE	PHE	GlY	ALA	LEU	SER	ASN
Li	4.26	0	12.8	8.51	0	10.6	8.51	2.13	10.6	4.26	2.13	2.13	0	2.13	2.13	0	0	Li	8.51	8.51	8.51
Na	3.42	0.72	14.5	12.3	1.11	16	2.83	3.73	6.07	4.01	3.63	3.03	1.49	0.59	2.26	1.8	0	Na	3.55	8.36	6.71
K	3.4	0.82	12.6	10.2	0.94	11	4.1	3.98	6.09	3.86	3.51	4.22	0.82	0.94	3.4	1.64	0	K	6.91	7.85	6.79
Rb	0	2.7	5.41	10.8	0	8.11	5.41	10.8	10.8	2.7	10.8	0	0	2.7	0	0	0	Rb	8.11	8.11	8.11
Cs	5.5	1.83	10.1	5.5	0	29.4	1.83	2.75	3.67	1.83	2.75	2.75	3.67	2.75	1.83	0	0	Cs	6.42	7.34	3.67
Mg	5.61	0.3	15.8	10.9	0.47	34.7	3.04	1.47	3.78	3.13	4.23	1.4	1.3	0.41	0.91	0.91	0	Mg	1.43	4.17	3.73
Ca	2.33	0.39	33.3	19.9	0.56	11.8	1.88	1.21	3.51	3.06	1.77	1.12	1.35	0.34	0.93	0.95	0	Ca	1.82	4.57	6.82
Sr	2.35	0	31.8	15.3	0	16.5	1.18	0	2.35	4.71	2.35	3.53	1.18	0	1.18	1.18	0	Sr	0	4.71	8.24
Ba	4.62	0	30.8	15.4	0	7.69	0	0	7.69	4.62	3.08	0	1.54	0	1.54	0	0	Ba	3.08	6.15	10.8
Mn	24.6	2.57	28.4	19.9	0	10.6	1.21	0.6	2.11	1.36	0.76	0.3	0.3	0	0.3	0.3	0	Mn	0.6	3.17	2.72
Fe	65.3	6.34	4.93	6.87	4.05	6.34	0.7	3.17	0.18	0.35	0	0	0.35	0	0	0	0	Fe	0	0.35	1.06
Co	43.9	3.8	17	16.7	1.46	9.94	0.29	0.59	1.17	0.59	0.59	0.29	0	0.29	0.59	0.29	0	Co	0.29	1.17	0.59
Ni	62.2	2	10.5	8.95	1.74	7.34	0.53	0	0.27	0.4	0.4	0.13	0.27	0.53	0.27	0	0	Ni	0.27	1.6	1.47
Cu	57.7	4.53	7.85	10.9	5.44	4.23	0.91	1.51	0.6	0.3	0.91	0.3	0	0	0.3	0	0	Cu	0.3	2.72	0.3
Zn	30.8	21.5	17.3	21.5	0.37	3.79	0.92	0.26	0.24	0.72	0.31	0.13	0.04	0.04	0.04	0.09	0	Zn	0.15	0.59	0.68
Pd	30.4	8.7	13	17.4	0	0	13	0	0	0	4.35	4.35	0	0	0	0	0	Pd	0	8.7	0
Cd	20.4	2.87	26.4	33.4	0.47	7.74	1.34	0.33	0.87	1	0.73	0.07	0.2	0.07	0.07	0	0	Cd	0.6	1.2	1.74
Pb	6.94	12.5	33.3	34.7	0	4.17	1.39	1.39	0	1.39	1.39	0	0	0	1.39	0	0	Pb	0	0	0
Al	0	0	25	25	0	0	0	0	25	25	0	0	0	0	0	0	0	Al	0	0	0
Ga	0	50	0	0	25	0	0	25	0	0	0	0	0	0	0	0	0	Ga	0	0	0
In	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	In	0	0	0
Sn	0	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Sn	0	0	0
Pt	18.6	6.83	0.62	3.11	39.8	11.8	12.4	0	0.62	1.24	2.48	0	0	0	0	0	0	Pt	0.62	0	1.24
Ag	22.9	14.3	2.86	5.71	40	2.86	0	2.86	0	0	0	2.86	2.86	0	0	0	0	Ag	0	2.86	0
Hg	10.9	65.2	1.37	1.56	2.73	2.15	0.78	1.95	1.17	0.59	1.37	0.78	0	0.59	0.59	0.78	0	Hg	1.37	2.34	1.95
W	25	50	0	0	0	0	25	0	0	0	0	0	0	0	0	0	0	W	0	0	0
Au	21.1	42.1	4.39	2.63	3.51	7.02	3.51	1.75	0.88	3.51	2.63	0	0.88	0.88	0	0	0	Au	0	0.88	3.51
Cr	66.7	0	33.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Cr	0	0	0

	HIS	CYS	ASP	GLU	MET	HOH	LYS	TYR	THR	GLN	ARG	VAL	PRO	TRP	ILE	PHE	GlY	ALA	LEU	SER	ASN
Li	1.00	-	1.18	1.10	-	1.92	1.00	1.00	1.00	1.25	1.00	1.00	-	1.00	1.00	1.00	-	1.50	1.00	1.00	1.00
Na	1.09	1.09	1.17	1.12	1.04	2.16	1.02	1.08	1.11	1.09	1.03	1.07	1.06	1.03	1.06	1.03	-	1.05	1.03	1.10	1.12
K	1.06	1.03	1.18	1.17	1.00	1.77	1.06	1.14	1.14	1.44	1.03	1.07	1.03	1.00	1.09	1.02	-	1.11	1.10	1.15	1.21
Rb	-	1.00	1.00	1.80	-	1.67	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	-	-	1.00	1.00	1.00	1.00
Cs	1.17	1.00	1.07	1.29	-	1.43	1.00	1.00	1.25	1.00	1.00	1.00	1.00	1.00	1.00	1.00	-	1.00	1.00	1.00	1.00
Mg	1.20	1.14	1.30	1.13	1.00	3.05	1.02	1.03	1.07	1.05	1.03	1.05	1.05	1.05	1.04	1.02	-	1.09	1.05	1.09	1.11
Ca	1.14	1.03	1.52	1.20	1.05	2.55	1.06	1.00	1.13	1.13	1.06	1.03	1.06	1.03	1.03	1.00	-	1.06	1.07	1.09	1.14
Sr	1.00	-	1.41	1.21	-	2.45	1.00	1.00	1.14	1.29	1.00	1.00	1.00	-	1.00	1.00	-	1.00	1.00	1.08	1.25
Ba	2.50	-	1.13	1.00	1.00	1.91	-	1.00	1.13	1.25	1.00	1.00	1.00	-	1.00	-	-	1.33	1.00	1.00	1.09
Mn	1.51	1.21	1.37	1.22	1.00	2.31	1.00	1.00	1.03	1.09	1.00	1.00	1.00	1.00	1.09	1.00	-	1.00	1.00	1.11	1.04
Fe	1.71	2.05	1.09	1.36	1.04	2.12	1.00	1.23	1.00	1.11	1.00	-	1.00	-	1.00	1.00	-	1.00	-	1.33	1.30
Co	1.53	1.59	1.21	1.20	1.00	2.29	1.00	1.00	1.00	1.00	2.00	1.00	-	1.00	1.00	1.00	-	1.00	1.00	1.18	1.00
Ni	1.59	1.46	1.17	1.15	1.06	2.21	1.00	1.00	1.00	1.00	1.14	1.00	1.00	1.25	1.50	1.00	-	1.00	1.00	1.12	1.14
Cu	1.63	1.39	1.14	1.13	1.64	1.56	1.00	1.36	1.00	1.00	1.00	1.00	-	-	1.00	-	-	1.00	1.00	1.00	1.25
Zn	1.39	2.87	1.17	1.18	1.00	1.74	1.03	1.03	1.03	1.00	1.07	1.00	1.00	1.00	1.13	1.00	-	1.00	1.09	1.02	1.09
Pd	1.00	1.00	1.67	1.00	1.00	1.44	1.20	-	-	1.00	1.00	1.00	-	-	-	-	-	-	-	1.00	-
Cd	1.20	1.75	1.13	1.19	1.00	1.98	1.00	1.20	1.09	1.00	1.05	1.00	1.00	1.00	1.00	1.00	-	1.00	1.00	1.07	1.00
Pb	1.14	1.50	1.54	1.18	-	1.42	1.00	1.00	1.00	1.00	1.00	1.00	-	-	1.00	1.00	-	1.00	1.00	-	1.00
Al	1.00	-	1.50	2.00	-	1.00	-	2.00	1.00	1.00	-	-	-	-	-	-	-	-	-	1.00	-
Ga	-	4.00	-	-	1.00	-	-	1.00	-	-	-	-	-	-	-	-	-	-	-	-	-
In	1.00	-	-	-	-	-	-	1.00	-	-	-	-	-	-	-	-	-	-	-	-	-
Sn	-	1.25	1.00	-	-	2.00	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Pt	1.00	1.36	1.00	1.00	1.05	1.79	1.00	-	1.00	1.00	1.00	-	-	-	-	-	-	1.00	1.00	-	1.00
Ag	1.33	1.83	1.33	1.00	2.05	1.00	-	1.00	-	1.00	1.00	1.00	1.00	-	-	-	-	-	-	1.00	-
Hg	1.18	1.13	1.12	1.06	1.06	1.28	1.00	1.00	1.00	1.00	1.10	1.00	1.00	1.00	1.00	1.00	-	1.00	1.00	1.07	1.00
W	1.00	1.00	1.00	1.00	-	1.00	1.00	-	-	-	-	-	-	-	-	-	-	-	-	1.00	-
Au	1.12	1.06	1.29	1.00	1.25	1.25	1.00	1.00	1.00	1.00	1.00	-	1.00	1.00	-	-	-	1.00	-	1.00	1.25
Cr	1.00	-	2.00	1.00	-	1.00	-	-	1.00	-	-	-	-	-	1.00	-	-	-	-	-	-