| HW 1 | Inorganic Materials <br> Chemistry | Name: |  |
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| Points: | C7780 | Due date: | 29.10 .2019 |
| Max. 100 points | Fall 2019 | A |  |

1. (20 pts) In the crystalline $\mathrm{Cu}_{2} \mathrm{O}$, oxygen atoms possess coordination number 4 . What is the coordination number of Cu ? Show how you arrived to the answer.
2. (10 pts) A unit cell has in general shape of a) cube b) tetrahedron c) parallelepiped
3. (20 pts) Give stoichiometric formulas for the cubic structures in the picture below. $\mathbf{a}=$ Heusler compound, $\mathbf{b}=$ Half-Heusler compound. Show how you arrived to the answer.

4. (25 pts) An octahedral structural unit $\mathrm{CoO}_{6}$ possesses following $\mathrm{Co}-\mathrm{O}$ bond distances (in $\AA$ ). Use Pauling Rules to establish whether the cobalt cation is in oxidation state 2+ or 3+. Use parameters $\mathrm{R}_{0}=1.692 \AA$ and $\mathrm{B}=0.30$.

2x Co1-O1 2.1033(12)
2x Co1-O2 2.0703(12)
2x Co1-O3 2.1204(12)
5. (25 pts) Use the Born-Landé equation and the appropriate Shannon-Prewitt radii (provided below) to calculate lattice energies ( $L_{0}$ ) for the following structures. Comment on results.

NaCl having the NaCl structure: $r_{\mathrm{Na}^{+}(\mathrm{CN} 6)}=1.16 \AA ; \mathrm{CCl}^{(\mathrm{CN}} \mathbf{( C )}=1.67 \AA$
NaCl having the CsCl structure: $r_{\mathrm{Na}^{+}}(\mathrm{CN} 8)=1.32 \AA ; r_{\mathrm{cl}}(\mathrm{CN} 6)=1.67 \AA$ (CN8 not avail.)

