APPENDIX C1

Physico-Chemical Properties and Chemical Classes of Metals Analyzed in the Applicability Domain of the LLNA

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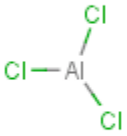
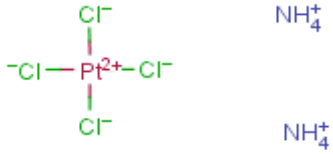
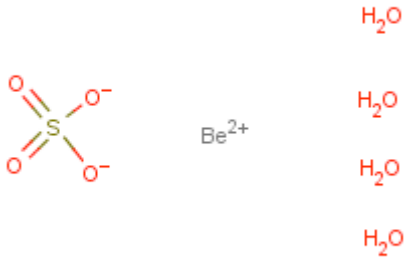
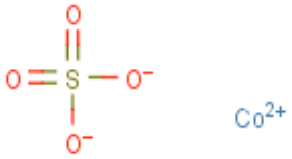
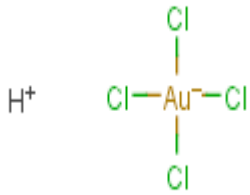
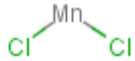
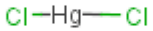
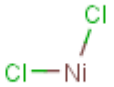
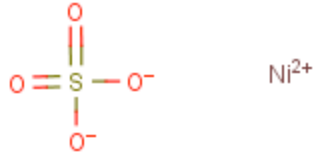
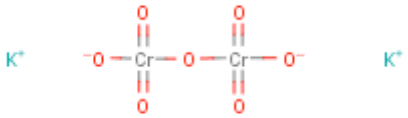
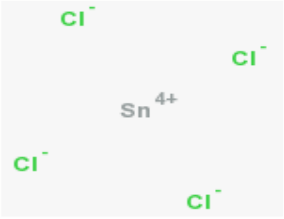
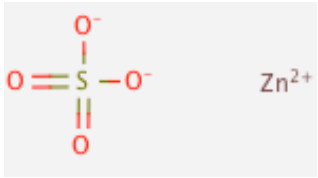
Physico-Chemical Properties – Metals (Sorted Alphabetically)

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow[1]	Physical Form	Chemical Class[2]	Structure[3]
Aluminum chloride	Aluminum chloride, anhydrous	7446-70-0	NA	NA	Solid	Inorganic Chemicals, Aluminum Compounds; Inorganic Chemicals, Chlorine Compounds	
Ammonium tetrachloroplatinate[5]	***Ammonium platinous chloride, Ammonium chloroplatinate***	***13820-41-2***	***372.97***	***0.47***	***Solid***	***Inorganic Chemicals, Platinum Compounds***	
Beryllium sulfate	***Beryllium sulfate tetrahydrate***	***7787-56-6***	***177.14***	***NA***	***Solid***	***Inorganic Chemicals; Metals; Salts***	
Cobalt chloride	***Cobaltous chloride***	***7646-79-9***	***129.84***	***0.85***	***Solid***	***Inorganic Chemicals; Metals; Salts***	
Cobalt (II) salts	NA	NA	NA	NA	Solid	Inorganic Chemicals; Metals; Salts	NA

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow[1]	Physical Form	Chemical Class[2]	Structure[3]
Cobalt sulfate	Cobaltous sulfate	10124-43-3	154.99	0.63	Solid	Inorganic Chemicals; Metals; Salts	
Copper chloride	***Cuprous chloride***	***7758-89-6***	***98.99***	***-0.26***	***NA***	***Inorganic Chemicals; Metals; Salts***	
Gold chloride	***Gold tetrachloride***	***16903-35-8***	***339.79***	***0.16***	***Solid***	***Inorganic Chemicals, Gold Compounds; Salts***	
Lead acetate	***Acetic acid, lead salt***	***15347-57-6***	***325.29***	***-0.08***	***Solid***	***Inorganic Chemicals; Metals; Salts***	
Manganese chloride	Manganese chloride, anhydrous	7773-01-5	125.84	0.85	Solid	Inorganic Chemicals, Manganese Compounds; Salts	

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow[1]	Physical Form	Chemical Class[2]	Structure[3]
Mercuric chloride	***Mercuric (II) chloride***	***7487-94-7***	***271.5***	***0.15***	***Solid***	***Inorganic Chemicals, Mercury Compounds; Salts***	
Nickel chloride	***Nickelous chloride***	***7718-54-9***	***129.6***	***0.05***	***Solid***	***Inorganic Chemicals; Metals; Salts***	
Nickel (II) salts	NA	NA	NA	NA	Solid	Inorganic Chemicals; Metals; Salts	NA
Nickel sulfate	***Nickel (II) sulfate***	***7786-81-4***	***154.76***	***-0.17***	***Solid***	***Inorganic Chemicals; Metals; Salts***	
Potassium dichromate	***PDC***	***7778-50-9***	***294.18***	***-2.24***	***Solid***	***Inorganic Chemicals, Chromium Compounds; Inorganic Chemicals, Potassium Compounds***	

Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow[1]	Physical Form	Chemical Class[2]	Structure[3]
Tin chloride	NA	1344-13-14	260.52	NA	Solid	Inorganic Chemicals, Tin Compounds; Salts	
Zinc sulfate	***Sulfuric acid, zinc salt; Zinc sulphate***	***7733-02-0***	***NA***	***NA***	***Solid***	Inorganic Chemicals, Zinc Compounds; Salts	

Bold, italicized text represent the 11 metals reported in the original LLNA Evaluation Report (ICCVAM 1999).
Abbreviations: CASRN=Chemical Abstract Services Registry Number; g/mol=Grams per mole; Kow=Octanol-water partition coefficient; NA=Not available.
[1]K_{ow} represents the octanol-water partition coefficient (expressed on log scale) obtained from the website: http://www.syrres.com/esc/est_kowdemo.htm..
[2]Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs, as developed by the National Library of Medicine at: http://www.nlm.nih.gov/mesh/meshhome.html.
[3]Chemical structures, based on CASRN, were obtained from ChemID available at: http://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp.