

Mineral Name	PDS4 Product ID	Chemistry
Albite (AL-I) <sup>a</sup>	albite_ali_frankspectrum	$\text{Na}_{0.89}\text{Ca}_{0.02}\text{K}_{0.01}\text{P}_{0.01}\text{Sr}_{0.01}\text{H}_{0.08}\text{Al}_{0.95}\text{Si}_{3.02}\text{O}_8$
Anorthite (AN-G) <sup>a</sup>	anorthite_ang_frankspectrum	$\text{Ca}_{0.79}\text{Na}_{0.15}\text{Mg}_{0.12}\text{Fe}^{2+}_{0.09}\text{Ti}_{0.01}\text{K}_{0.01}\text{H}_{0.19}(\text{Al}_{1.63}\text{Fe}^{3+}_{0.03})\text{Si}_{2.15}\text{O}_8$
Augite (Harcourt) <sup>b</sup>	augite_harcourt_frankspectrum	$\text{Ca}_{0.94}\text{Mg}_{0.68}\text{Na}_{0.03}\text{Mn}_{0.01}\text{Al}_{0.02}\text{Fe}_{0.31}\text{Si}_{2.01}\text{O}_6$
Bytownite (Crystal Bay) <sup>b</sup>	bytownite_cb_frankspectrum	$\text{Ca}_{0.65}\text{Na}_{0.33}\text{Mg}_{0.01}\text{K}_{0.01}\text{Al}_{1.62}\text{Fe}_{0.02}\text{Si}_{2.35}\text{O}_8$
Diopside (Herschel) <sup>b</sup>	diopside_herschel_frankspectrum	$\text{Ca}_{0.96}\text{Mg}_{0.89}\text{Na}_{0.03}\text{Al}_{0.12}\text{Fe}_{0.06}\text{Si}_{1.95}\text{O}_6$
Enstatite (Zen-1) <sup>c</sup>	enstatite_zen1_frankspectrum	$\text{Mg}_{1.81}\text{Ca}_{0.01}\text{Mn}_{0.01}\text{Al}_{0.01}\text{Fe}_{0.18}\text{Si}_{1.99}\text{O}_6$
Fe-metal (AA-70) <sup>d</sup>	fe-metal_aa70_frankspectrum	Fe (99.5%)
Forsterite (Globe) <sup>b</sup>	forsterite_globe_frankspectrum	$\text{Mg}_{1.82}\text{Fe}_{0.18}\text{Ni}_{0.01}\text{SiO}_4$
Forsterite (San Carlos) <sup>b</sup>	forsterite_sc_frankspectrum	$\text{Mg}_{1.81}\text{Fe}_{0.19}\text{Ni}_{0.01}\text{SiO}_4$
Graphite (AA-30) <sup>d</sup>	graphite_aa30_frankspectrum	C (99%)
Hectorite (SHCa-1) <sup>c</sup>	hectorite_shca1_frankspectrum	$\text{Ca}_{4.29}\text{Mg}_{3.90}\text{Na}_{0.42}\text{Al}_{0.14}\text{Fe}^{2+}_{0.04}\text{K}_{0.03}\text{P}_{0.01}\text{Li}_{1.50}\text{F}_{1.41}\text{Si}_{5.94}\text{H}_4\text{O}_{22}$
Hematite (SA-500G) <sup>d</sup>	hematite_sa500g_frankspectrum	$\text{Fe}_2\text{O}_3$ (>96%)
Ilmenite (AA-30) <sup>d</sup>	ilmenite_aa30_frankspectrum	$\text{FeTiO}_3$ (>99.8%)
Kaolinite (KGa-1b) <sup>c</sup>	kaolinite_ka1b_frankspectrum	$\text{Al}_{4.07}\text{K}_{0.01}\text{P}_{0.01}\text{Fe}^{2+}_{0.01}\text{Ti}_{0.09}\text{Fe}^{3+}_{0.01}\text{Si}_{3.84}\text{H}_8\text{O}_{14}$
Labradorite (ARSAA) <sup>c</sup>	labradorite_arsaa_frankspectrum	$(\text{Ca}_{0.57}\text{Na}_{0.44}\text{Fe}_{0.02}\text{K}_{0.01})\text{Al}_{1.62}\text{Si}_{2.38}\text{O}_8$
Labradorite (Chihuahua) <sup>b</sup>	labradorite_chihuahua_frankspectrum	$(\text{Ca}_{0.59}\text{Na}_{0.39}\text{Fe}_{0.01}\text{Mg}_{0.01}\text{K}_{0.02})\text{Al}_{1.60}\text{Si}_{2.39}\text{O}_8$
Ca-montmorillonite (STx-1b) <sup>c</sup>	ca-montmorillonite_stx1b_frankspectrum	$(\text{Ca}_{0.19}\text{Na}_{0.06}\text{K}_{0.01}\text{P}_{0.01}\text{F}_{0.03})[\text{Al}_{2.15}\text{Ti}_{0.02}\text{Fe}^{3+}_{0.06}\text{Fe}^{2+}_{0.10}\text{Mg}_{0.63}]\text{Si}_{7.98}\text{O}_{20}(\text{OH}_{1.90})_4$
Na-montmorillonite (SWy-3) <sup>c</sup>	na-montmorillonite_swy3_frankspectrum	$(\text{Ca}_{0.23}\text{Na}_{0.38}\text{K}_{0.09}\text{F}_{0.04}\text{Fe}^{2+}_{0.03}\text{P}_{0.03})[\text{Al}_{2.94}\text{Ti}_{0.01}\text{Fe}^{3+}_{0.32}\text{Mg}_{0.58}]\text{Si}_{7.99}\text{O}_{18}(\text{OH})_4$
Nontronite (NAu-2) <sup>c</sup>	nontronite_nau2_frankspectrum	$\text{Al}_{0.53}\text{Fe}^{3+}_{3.74}\text{Mg}_{0.07}\text{Ca}_{0.38}\text{Na}_{0.03}\text{Si}_{7.57}\text{H}_4\text{O}_{22}$
Oldhamite (AA-14) <sup>d</sup>	oldhamite_aa14_frankspectrum	CaS (99.9%)
Palygorskite (PFI-1) <sup>c</sup>	palygorskite_pfi1_frankspectrum	$\text{Al}_{1.63}\text{Ti}_{0.05}\text{Fe}^{2+}_{0.04}\text{Fe}^{3+}_{0.30}\text{Mg}_{2.03}\text{Ca}_{0.28}\text{Na}_{0.01}\text{Mn}_{0.01}\text{K}_{0.14}\text{P}_{0.45}\text{F}_{0.23}\text{Si}_{8.11}\text{H}_{4.00}\text{O}_{22}$
Phlogopite (Mica-Mg) <sup>a</sup>	phlogopite_micamg_frankspectrum	$\text{Al}_{0.05}\text{Ti}_{0.22}\text{Fe}^{2+}_{1.03}\text{Fe}^{3+}_{0.27}\text{Mg}_{5.55}\text{Mn}_{0.04}\text{Ca}_{0.02}\text{Na}_{0.04}\text{K}_{2.33}\text{P}_{0.01}\text{Si}_{6.99}\text{H}_{2.54}\text{O}_{24}$
Pyrite (SA-25G) <sup>d</sup>	pyrite_sa25g_frankspectrum	$\text{FeS}_2$ (99.8%)

Serpentine (SMS-16) <sup>c</sup>	serpentine_sms16_frankspectrum	$\text{Mg}_{2.83}\text{Fe}^{3+}_{0.02}\text{Si}_{2.07}\text{H}_{4.01}\text{O}_9$
Serpentine (UB-N) <sup>a,f</sup>	serpentine_ubn_frankspectrum	$\text{Mg}_{2.59}\text{Al}_{0.17}\text{Fe}^{2+}_{0.11}\text{Fe}^{3+}_{0.20}\text{Mn}_{0.01}\text{Ca}_{0.06}\text{Na}_{0.01}\text{P}_{0.01}\text{Si}_{1.94}\text{H}_{3.56}\text{O}_9$
Spinel (ARSAA) <sup>c</sup>	spinel_arsaa_frankspectrum	$\text{Al}_{1.98}\text{Mg}_{0.99}\text{Ba}_{0.03}\text{Fe}^{2+}_{0.01}\text{O}_4$
Zinnwaldite (ZW-C) <sup>a</sup>	zinnwaldite_zwc_frankspectrum	$\text{Ca}_{0.06}\text{Na}_{0.10}\text{K}_{1.48}\text{Al}_{3.26}\text{Fe}^{3+}_{0.15}\text{Fe}^{2+}_{0.92}\text{Mg}_{0.04}\text{Mn}_{0.12}\text{P}_{0.02}\text{Ti}_{0.01}$ $\text{Si}_{8.10}\text{O}_{24}\text{H}_{1.46}$

<sup>a</sup>CRPG standard; <sup>b</sup>Byrne et al. (2015); <sup>c</sup>Our electron microprobe analysis; <sup>d</sup>synthesized (AA from Alfa Aesar; SA from Sigma-Aldrich); <sup>e</sup>CMS standard;

<sup>f</sup>UB-N is from the “2015 lot” and has a lizardite structure (Gayk & Kleinschrodt, 2000; Hallett et al., 2021).