DISCOVERY OF KAITIANITE, $Ti^{3+}{}_2Ti^{4+}O_5$, IN ALLENDE: A NEW REFRACTORY MINERAL FROM THE SOLAR NEBULA.

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Introduction: The Allende meteorite, fell in Mexico on February 8, 1969, is a CV3 carbonaceous chondrite. It is often called the best-studied meteorite in history. Fifty years after it fell, this meteorite continues to be source of new discoveries. Allende has yielded 19 new minerals since 2007 [e.g., 1-4], including 11 ultrarefractory or refractory phases. Each new mineral adds a new puzzle piece toward our understanding of nebular or parent body processes in the early solar system. Reported here is the discovery of kaitianite, $Ti^{3+}{}_2Ti^{4+}O_5$, a refractory titanium oxide from the solar nebula – the latest new mineral in Allende.

During an ongoing nanomineralogy investigation of the Allende CV3 carbonaceous chondrite, new mineral kaitianite, $Ti^{3+}{}_2Ti^{4+}O_5$ with a *C*2/*c* V_3O_5-type structure, was identified in section USNM 3510-5. Field-emission scanning electron microscope (SEM), energy-dispersive X-ray spectroscopy (EDS), electron back-scatter diffraction (EBSD) and electron probe microanalyzer (EPMA) were used to characterize kaitianite and associated phases. Fine-grained Ti_3O_5 phase was observed in a chondrite matrix clast in the Nilpena polymict ureilite [5]. Synthetic Ti_3O_5 with the *C*2/*c* V_3O_5 structure is reported as γ-Ti_3O_5 [6,7]. Kaitianite, the natural occurrence of $Ti^{3+}{}_2Ti^{4+}O_5$ with the *C*2/*c* V_3O_5 structure as a new mineral in Allende, has been approved by the IMA-CNMNC (IMA 2017-078a) [8]. The name is after two Chinese words "Kai Tian", meaning *creating the heaven* / *the sky*, from the story of "Pan Gu Kai Tian" in the ancient Chinese mythology. Pan Gu, the giant, created the world by separating the heaven and earth from an egg-shaped chaos in the beginning. Panguite ($(Ti^{4+},Sc,Al,Mg,Zr,Ca)_{1.8}O_3$; IMA 2010-057 [1]) was named after "Pan Gu" in allusion to the mineral with an ultrarefractory origin being among the first solid materials in the solar system. Kaitianite ($Ti^{3+}{}_2Ti^{4+}O_5$) is also a refractory phase formed in the solar nebula.

Occurrence, Chemistry, and Crystallography: Kaitianite occurs as two crystals, 0.3~0.6 μm × 3.6 μm and 0.2 μm × 1.1 μm, within one irregular grain in contact with tistarite and rutile, along with Ti^{3+}-bearing corundum, Ti^{3+},Al,Zr-oxide, and Ti-bearing xifengite grains in a crack in the Allende matrix. These grains are likely from the cluster of refractory phases identified in a chondule in USNM 3510-6, where Ti^{3+}-bearing corundum grains, mullite, khamrabaevite (TiC) and the type tistarite (Ti_2O_3; IMA 2008-016) were first identified [9,10]. USNM 3510-5 and USNM 3510-6 are series cut thin sections. The O-isotope analyses of two corundum grains in the cluster in USNM 3510-6 reveal that the grains have compositions well above the terrestrial fractionation line but on the CCAM line [10], which is consistent with formation or alteration in an O^{16}-depleted reservoir.

The chemical composition of type kaitianite by low-voltage EPMA (WDS) is (wt%) Ti_2O_3 56.55, TiO_2 39.29, Al_2O_3 1.18, MgO 1.39, FeO 0.59, V_2O_3 0.08, sum 99.07, showing an empirical formula (based on 5 O atoms *pfu*) of $(Ti^{3+}{}_{1.75}Al_{0.05}Ti^{4+}{}_{0.10}Mg_{0.08}Fe_{0.02})(Ti^{4+}{}_{1.00})O_5$, with Ti^{3+} and Ti^{4+} partitioned, based on stoichiometry. The end-member formula is $Ti^{3+}{}_2Ti^{4+}O_5$. The EBSD patterns of kaitianite can be indexed only by the *C*2/*c* V_3O_5-type structure and give a perfect fit by the synthetic γ-Ti_3O_5 cells from [6,7], with a mean angular deviation of 0.33º, revealing a = 10.115 Å, b = 5.074 Å, c = 7.182 Å, β = 112º, V = 341.77 Å^3, and Z = 4.

Associated Ti^{3+},Al,Zr-oxide is a new Zr-rich ultrarefractory phase from Allende. It has an empirical formula (based on 3 O atoms *pfu*) of $(Ti^{3+}{}_{1.16}Al_{0.57}Zr_{0.11}Si_{0.07}Mg_{0.03})_{\sum 1.95}O_3$ and a general formula of $(Ti^{3+},Al,Zr,Si,Mg)_{1.95}O_3$. Its crystal structure is related to panguite-kangite-type but highly-ordered, as revealed by EBSD.

Origin and Significance: Kaitianite ($Ti^{3+}{}_2Ti^{4+}O_5$) is γ-Ti_3O_5, the Ti-analog of oxyvanite (V_3O_5), a new member of the oxyvanite group. Kaitianite is a refractory titanium oxide, joining other Ti-rich refractory minerals from carbonaceous chondrites including perovskite, Al,Ti-diopside, tistarite, rutile, grossmanite, davisite, panguite, kangite, anosovite, paqueite, zirkelite, tazheranite, rubinite, and Ti^{3+},Al,Zr-oxide.

Multiple refractory phases (tistarite, corundum, kaitianite, Ti^{3+},Al,Zr-oxide, khamrabaevite) are potentially useful as probes of their formation environments. These grains either indicate or are consistent with extremely reducing conditions. Kaitianite is a first solar titanium oxide with structurally essential Ti^{3+} and Ti^{4+}, probably crystallized from a refractory melt or condensed from a gaseous reservoir under highly-reduced conditions.

References: [1] Ma C. et al. 2012. *American Mineralogist* 97:1219–1225. [2] Ma C. et al. (2014) *American Mineralogist* 99:654–666. [3] Ma C. and Krot A.N. (2018) *American Mineralogist* 103:1329–1334. [4] Ma C. and Beckett J.R. 2018. *American Mineralogist* 103:1918–1924. [5] Brearley A.J. 1993. *Meteoritics* 28:590–595. [6] Hong S.H. and Asbrink S. 1982. *Acta Crystallographica B* 38:2570–2576. [7] Tanaka K. et al. 2015. *Crystal Growth & Design* 15:653–657. [8] Ma C. 2018. *Mineralogical Magazine* 82:450. [9] Ma C. and Rossman G.R. 2009. *American Mineralogist* 94:841–844. [10] Ma et al. 2009. *LPSC* 40:A2138.