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The atomic arrangement of merrillite from the Fra Mauro Formation, Apollo 14 lunar mission: The first structure of merrillite from the Moon

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ABSTRACT

The atomic arrangement of lunar merrillite has been refined to $R = 0.0452$ in $R3c$ using X-ray diffraction data recorded on a CCD detector; previous attempts at structure solution using a point detector were not successful because of the poorly crystallized nature of the lunar material. The atomic arrangement of merrillite has a structural unit of $[(Mg,Fe)(PO_4)_6]_2^{16-}$ that forms a "bracelet-and-pinwheel" unit that is common in hexagonal-closest-packed layers. The individual structural units are not polymerized and exist in layers at $z = 1/6$, 1/3, 1/2, 2/3, and 5/6. In lunar merrillite, the $[(Mg,Fe)(PO_4)_6]_2^{16-}$ structural units are linked by a $[(Ca,REE)_{18}Na_2(PO_4)_2]^{32+}$ interstitial complex, formed of $Ca1O_8$, $Ca2O_8$, $Ca3O_8$, NaO_6, and $P1O_4$ polyhedra.

There has long been speculation regarding the relationship between merrillite and terrestrial whitlockite, and the solution of the Fra Mauro merrillite atomic arrangement allows the characterization of the lunar phase. Lunar merrillite and terrestrial whitlockite have largely similar atomic arrangements, but the phases differ due to the presence or absence of hydrogen. In whitlockite, H is an essential element and allows the charge balance. Hydrogen is incorporated into the whitlockite atomic arrangement by disordering one of the phosphate tetrahedra and forming a $PO_3(OH)$ group. Lunar merrillite is devoid of hydrogen, and thus no disordered tetrahedral groups exist. Charge balance for substituents Y and REE (for Ca) is maintained by Si ↔ P tetrahedral substitution and □ ↔ Na at the Na site. The structure solution demonstrates the effectiveness of the CCD detector in unraveling previously intractable diffraction data and urges that previously analyzed lunar material be reexamined using this instrumentation.

Keywords: Merrillite, Moon, atomic arrangement, chemistry