CRYSTAL STRUCTURE OF CHLADNIITE, $Na_2CaMg_7(PO_4)_6$, FROM CARLTON (IIICD) IRON METEORITE. Ian M. Steele, Department of Geophysical Sciences, University of Chicago, 5734 S. Ellis Ave., Chicago IL 60637.

A new phosphate occurring in the Carlton (IIICD) iron meteorite has been described [1] with a composition and cell parameters reminescent of terrestrial fillowite [2]. This phase has been named chladniite and has been approved by the Committee on New Minerals. A single crystal structure refinement has been completed confirming the fillowite structure as reported here. In addition, a third composition has been reported [5] from El Sampal (IIIAB) analogous to terrestrial johnsomervilleite and its structure determination is in progress.

Compositions: The ideal compositions of the three phases are:

Fillowite -	$Na_2\,Ca\,Mn_7(PO_4)_6$	,occurs in terrestrial pegmatites
Chladniite -	$Na_2\,Ca\,Mg_7(PO_4)_6$	,only one occurence in Carlton IIICD
Johnsomervilleite-	$Na_2\,Ca\,Fe_7(PO_4)_6$	,occurs terrestrially and in meteorites

The structure of terrestrial fillowite (composition based on structure: $Na_{1.95}Ca_{0.77}Mn_{5.94}Fe_{1.34}(PO4)_6$) has been determined [2] while that of an isostructural synthetic orthophosphate phase, $Na_4Ca_4Mg_{21}(PO_4)_{18}$, has also been determined [4]. This composition ($Na_{1.33}Ca_{1.33}Mg_7(PO4)_6$) is similar to that of Carlton chladniite [1] ($Na_{1.77}Ca_{0.98}Si_{0.08}Mg_{6.96}Fe_{0.26}Mn_{0.04}(P_{0.98}O_4)_6$) except with respect to Ca and Na.

Experimental: Single crystal x-ray intensities were obtained with a four circle diffractometer using CuKα radiation. Cell parameters were obtained by least squares refinement using 20 centered diffractions, each the average of automatic centering of eight equivalent settings. The resulting cell parameters are: a = 14.967±0.002, c = 42.595±0.004Å, $\beta = 120^o$ with space group R3 . A total of 5651 diffractions gave 1880 independent diffractions after averaging. Full-matrix isotropic refinement using initial parameters of fillowite [2] and varying site occupancy gave a final R-factor of 0.04. Structural parameters, isotropic temperature factors, and occupancies are in Table 1.

Discussion: Chladniite is isostructural with fillowite. It is anticipated the meteoritic johnsomervilleite will also be isostructural based on the similar composition and cell parameters of terrestrial johnsomervilleite [3] to those of fillowite. The site occupancy refinement of chladniite shows that the 8-coordinated site labeled Ca is actually partially occupied by Na both in terrestrial fillowite [2] (Table 2) and in chladniite in an almost identical Ca:Na ratio near 0.67:0.33. This may be fortuitous but may represent partial ordering violating the R3 space group. This mixed occupancy also can explain the consistent analytical results giving high Na and low Ca relative to the above ideal stoichiometry (E. Olsen, personal comm.). The Na(1) site appears partially vacant in both synthetic and natural chladniite.

References: [1] McCoy et al. (1993) Meteoritics **2 8**, 394; [2] Araki, T. and Moore, P.B. (1981) Am. Mineral. **6 6**, 827-842; [3] Livingstone, (1980) Min. Mag **4 3**, 833-836; [4] Domanskii, A.I. et al. (1982) Sov. Phys. Crystallogr. **2 7**, 535-537; [5] Olsen, E. and Steele, I. (1993) Meteoritics **2 8**, 415.

Acknowledgements: NASA NAGW-3416 for financial support, E. Olsen for comments, and J. Pluth for data collection and refinement.

CRYSTAL STRUCTURE OF CHLADNIITE ..... : Steele, I.M.

TABLE 1. POSITIONAL AND ISOTROPIC DISPLACEMENT PARAMETERS FOR CHLADNIITE.

Site	Occupancy	*x*	*y*	*z*	$^{*}U_{eq}$
M(1)	1.00 Ca	0.0	0.0	0.0	0.022(2)
M(2)	1.00 Mg	0.0	0.0	0.5	0.005(3)
M(3)	1.00 Mg	0.0	0.0	0.1039(3)	0.013(2)
M(4)	1.00 Mg	0.0	0.0	0.3248(3)	0.014(2)
M(5)	1.00 Mg	0.0	0.0	0.3966(3)	0.010(2)
M(6)	1.00 Mg	0.4304(3)	0.2529(3)	0.0521(2)	0.012(1)
M(7)	1.00 Mg	0.1113(3)	0.5728(3)	0.0392(2)	0.010(1)
M(8)	1.00 Mg	0.0022(3)	0.3229(3)	0.0819(1)	0.012(1)
M(9)	1.00 Mg	0.2599(3)	0.3276(3)	0.0862(1)	0.009(1)
M(10)	1.00 Mg	0.5733(3)	0.0796(3)	0.1235(2)	0.015(1)
M(11)	1.00 Mg	0.2222(3)	0.1092(3)	0.1341(2)	0.015(1)
Na(1)	0.81 Na	0.0	0.0	0.1760(4)	0.017(6)
Na(2)	1.00 Na	0.0	0.0	0.2481(3)	0.014(3)
Na(3)	1.00 Na	0.0790(4)	0.4278(4)	0.1650(2)	0.028(2)
Ca	0.69 Ca, 0.31 Na	0.2657(2)	0.2923(2)	0.0008(1)	0.019(2)
P(1)		0.1895(3)	0.4342(3)	0.0283(1)	0.011(1)
P(2)		0.5327(3)	0.1164(3)	0.0382(1)	0.011(1)
P(3)		0.5441(3)	0.0926(3)	0.1991(1)	0.013(1)
P(4)		0.2201(3)	0.1259(3)	0.2105(1)	0.012(1)
P(5)		0.2247(3)	0.4621(3)	0.2226(1)	0.014(1)
P(6)		0.4674(3)	0.2154(3)	0.2782(1)	0.014(1)
O(1)		0.1619(6)	0.3829(6)	0.9956(3)	0.012(2)
O(2)		0.2532(6)	0.5532(6)	0.0260(3)	0.013(3)
O(3)		0.2554(6)	0.3973(6)	0.0459(3)	0.012(3)
O(4)		0.0893(6)	0.4106(6)	0.0448(3)	0.010(2)
O(5)		0.4570(6)	0.1299(6)	0.0591(3)	0.014(3)
O(6)		0.5547(6)	0.0337(6)	0.0511(3)	0.013(3)
O(7)		0.6382(6)	0.2159(6)	0.0385(3)	0.009(3)
O(8)		0.4893(6)	0.0925(6)	0.0044(3)	0.016(3)
O(9)		0.5431(6)	0.0347(6)	0.1697(3)	0.016(3)
O(10)		0.6318(6)	0.2057(6)	0.1982(2)	0.009(2)
O(11)		0.4402(5)	0.0910(6)	0.2025(2)	0.008(3)
O(12)		0.5495(6)	0.0366(6)	0.2290(3)	0.011(3)
O(13)		0.2353(6)	0.0866(7)	0.1786(3)	0.031(3)
O(14)		0.1280(5)	0.1427(6)	0.2090(3)	0.010(3)
O(15)		0.8919(6)	0.2363(5)	0.1145(3)	0.008(2)
O(16)		0.1985(6)	0.0410(6)	0.2348(3)	0.014(2)
O(17)		0.2668(6)	0.5282(6)	0.1936(3)	0.016(3)
O(18)		0.1035(5)	0.3969(5)	0.2206(2)	0.009(2)
O(19)		0.2553(6)	0.3778(6)	0.2234(3)	0.011(3)
O(20)		0.2542(6)	0.5244(6)	0.2531(3)	0.015(3)
O(21)		0.5290(7)	0.2449(6)	0.2482(3)	0.025(3)
O(22)		0.3778(6)	0.1011(6)	0.2737(3)	0.011(3)
O(23)		0.4176(6)	0.2828(6)	0.2830(2)	0.014(3)
O(24)		0.5258(7)	0.2149(6)	0.3073(3)	0.031(3)

$^{*}U_{eq}$ is defined as $\frac{1}{3} \sum_{i=1}^{3} \sum_{j=1}^{3} U_{ij} a_i^{*} a_j^{*} (\mathbf{a}_i \cdot \mathbf{a}_j)$

TABLE 2. SITE OCCUPANCIES OF OTHER REFINEMENTS.

Fillowite[2]	Orthophosphate[4]
0.62 Mn,0.38 Ca	1.00 Ca
1.00 Mn	1.00 Mg
1.00 Fe	1.00 Mg
1.00 Fe	1.00 Mg
1.00 Mn	1.00 Mg
1.00 Mn	1.00 Mg
1.00 Mn	1.00 Mg
0.67 Fe, 0.33 Mn	1.00 Mg
1.00 Mn	1.00 Mg
1.00 Mn	1.00 Mg
1.00 Mn	1.00 Mg
0.91 Na, 0.09 Ca	-
0.90 Na, 0.10 Ca	1.00 Na
1.00 Na	1.00 Na
0.65 Ca, 0.35 Na	1.00 Ca