MODAL MINERALOGY OF HED ACHONDRITE METEORITES BY RIETVELD REFINEMENT.

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Introduction: Knowledge of the proportions of the constituent minerals in a rock - the modal mineralogy - provides insight into its formation and alteration history. For meteorites, this information is often lacking or where available, based on analysis of a limited volume of material such as a single petrographic thin section. Powder X-ray diffraction, which interrogates a relatively large and homogenized sample, can provide a more representative view of the modal mineralogy of a meteoritic sample. Several methods have been applied to quantify mineral abundances from X-ray diffraction data [1,2]. In this study, we applied Rietveld refinement to synchrotron powder X-ray diffraction data to determine the detailed mineral modes of achondritic meteorites. We conducted a survey of the howardite, eucrite, and diogenite (HED) suite including NWA 1942, NWA 1943, Millbillillie, NWA 1836, Talampaya, NWA 6477, JaH 626, Tatahouine, and NWA 6013.

Methods: Powder X-ray diffraction data were collected from meteorite samples ground to 5 μm were loaded in borosilicate glass capillaries at Beamline i-11 at the Diamond Light Source using white radiation with 0.824883 Å wavelength. Rietveld refinement uses a model of the incident radiation, the instrument, and the structure and composition of the scattering matter to create a simulated diffraction pattern. The simulated diffraction pattern is then compared with the measured X-ray diffractogram for that sample, and nonlinear least-squares optimization of the model parameters (instrumental parameters, abundance and crystallographic parameters of the mineral(s) present) carried out to find the best fit of the model parameters to the X-ray diffractogram [3]. Rietveld refinement of X-ray diffraction patterns was performed using BrukerAXS TOPAS4 ver. 4.2 software, in fundamental parameters (FP) mode. Because the purpose of Rietveld refinement in this study is the quantification of the mineralogy of the meteorite samples, the atomic co-ordinates and compositions of the minerals were not refined. Instead, 'standard' crystal structures and compositions were used, with chemical compositions fixed to average values for the meteorites in question where available, or to reasonable values for the class of meteorite where average values were not available.

Results: Mineral modes for the major phases (plagioclase, pigeonite, augite, orthopyroxene and olivine) and weighted profile residuals (a measure of goodness of fit in Rietveld refinement [3]) are shown in Table 1.

sample	plag	pig	aug	opx	olv	Rwp
NWA 1942	35	34	n.d.	30	1	5.41
NWA 1943	43	27	15	15	n.d.	5.04
NWA 5751	28	13	7	50	1	5.64
NWA 6477	54	33	13	n.d.	n.d.	6.55
Talampaya	65	32	1	n.d.		9.32
JaH 626	40	59	n.d.	n.d.	n.d.	5.95
Millbillillie	49	24	12	14	n.d.	4.6
NWA 1836	28	55	n.d.	17	n.d.	6.28
Tatahouine	n.d.	n.d.	n.d.	97	Tr	8.83
NWA 6013	7	n.d.	n.d.	65	27	6.07

Table 1: Refined abundances of major minerals. n.d. = not detected. Rwp = weighted profile residual. Errors in the mineral abundances from the covariance matrix of the least-squares fit are less than ~1% (2σ).

Integration with spectral analysis: Combining the modal mineralogy with spectral parameters previously measured for these HED meteorites [4] reveals several spectral-compositional trends. The ratio of orthopyroxene to total pyroxene displays a trend (Figs 1-2) with both band I and band II centers qualitatively similar to that of the widely-used Band Area Ratio vs. Band I center plot [5], consistent with a dependence of band center locations on average pyroxene chemistry witch is related to the relative proportions of diogenite and eucrite materials. Band center locations also display a systematic variation with respect to the proportions of augite and pigeonite (Figs. 4-5), which may enable interpretation of the cooling history of HED-like asteroidal surface rocks.

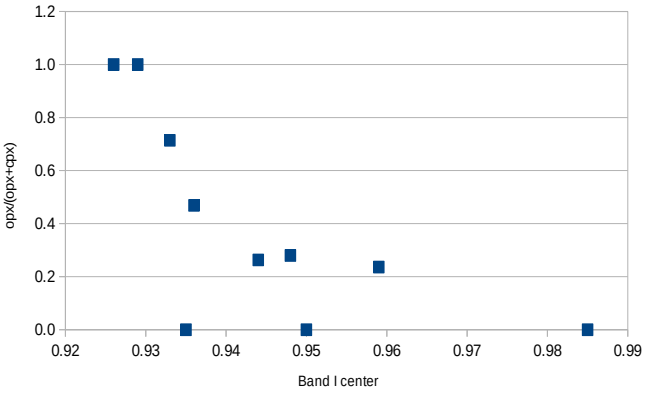

Figure 1: Ratio of orthopyroxene to total pyroxene as a function of band I center wavelength.

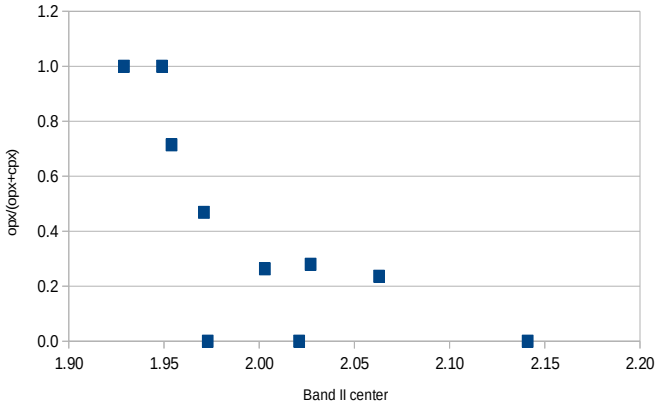

Figure 2: Ratio of orthopyroxene to total pyroxene as a function of band II center wavelength.

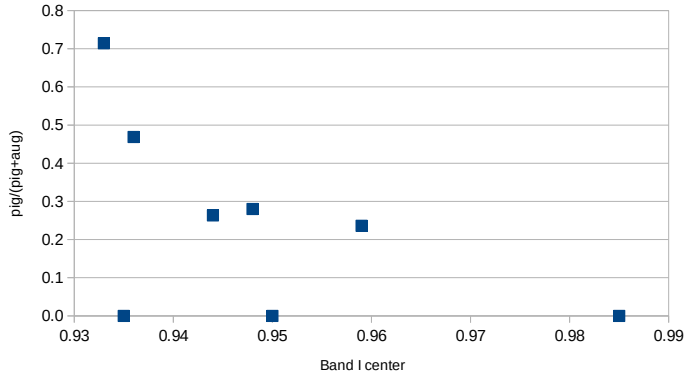

Figure 3: Ratio of pigeonite to total calcic pyroxene as a function of band I center wavelength.

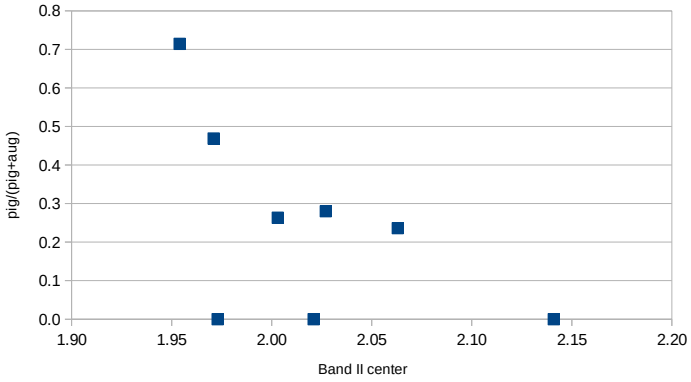

Figure 4: Ratio of pigeonite to total calcic pyroxene as a function of band II center wavelength.

References: [1] Bland et al 2004 MAPS 39(1) 3-16; -[2] Izawa et al 2010 MAPS 45(4) 675-698; [3] Rietveld 1969 J. Appl. Cryst. 2 65-71; [4] Cloutis et al., 2013 Icarus 223(2) 850-877; [5] Gaffey et al. (1993) Icarus 106, 573.