Fourier Transform Infrared Spectroscopic Characterization of Dergaon H5 Chondrite: Evidence of Aliphatic Organic Compound

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Abstract: We report the spectroscopic investigations of the Dergaon H5 chondrite in the mid infrared region. Compositional characterization is presented with the help of X-ray fluorescence (XRF) spectroscopy. Fourier transform infrared (FTIR) spectroscopic study of Dergaon H5 chondrite exhibits prominent absorption band in 800-1100 cm⁻¹ region originating from valance vibration of SiO₄ tetrahedra. Particular interest is directed towards the presence of trace of organic compound in the spectral region around 2800-3000 cm⁻¹, which is generally not observed in the meteorites of this type. The FTIR approach shows the organic material present in Dergaon is aliphatic functional groups CH_2 and CH_3 . [Nature and Science. 2009;7(5):45-51]. (ISSN: 1545-0740).

Key words: Dergaon H5 chondrite; organic compounds; infrared spectroscopy

1. Introduction

Meteorites are some of the oldest remnants of the solar system available for laboratory studies. They are classified on the basis of their mineralogy, structure and chemical compositions (Oura et al 2002; Randa et al 2003; Ebihara et al 1996; Larimer 1971). The general mineral groups in meteorites are: silicates, metal, sulfides, oxides, phosphates and carbon compounds. The main classes of meteorites are: (i) stony meteorites constituting 92.8% of all meteorites, (ii) stony iron meteorites constituting nearly 1.5% and (iii) iron meteorites with abundance of 5.7%. Generally majority of primitive meteorites have small round mass of olivine or pyroxene called chondrules, they are commonly named chondrites. Chondritic meteorites are the oldest and most primitive rocks in the solar system. The primary divisions of chondrite classification are the carbonaceous, ordinary, and enstatite classes. The chondrites are the most numerous meteorite group, accounting for 87% of all meteorites observed to fall. The largest group of chondritic meteorites is known as the ordinary chondrites, account for 80% of all known meteorites (Philip et al 2000). Three subgroups of ordinary chondrites are identified, H group (high iron), L group (low iron), and LL group (low total iron, low metal). There is some evidence that carbon is frequently associated with Fe-Ni metal (McKinley et al 1981; Scott et al 1988; Brearley 1990; Cronin et al 1988), and carbon of unknown chemical form has been identified at the surface of metal and troilite grains in ordinary chondrites (Makjanic et al 1993). In unequilibrated ordinary chondrites (UOCs), the carbon content usually ranges from 0.2 to 0.6%, but reaches 1% in a few cases (Smail et al 2000). A numbers of authors suggested that the volatile organic compounds including aldehydes, amides, amines, mono and di-carboxylic acids, aliphatic and aromatic hydrocarbons, heterocyclic aromatics, hydroxy acids, ketones, phosphonic and sulfonic acids, fatty acids, purines, pyrimidines are present in meteorites (Cronin and Chang 1993; Palme 2000). These organic molecules are generally believed to be abiogenic (Cronin et al 1988), have been produced by chemical rather than biologic processing. Exogenous delivery of organics to the earth's surface could have been an important source of these molecules on the prebiotic earth.

The FTIR spectroscopy presents the advantage of being non-destructive technique; therefore, it is highly appreciated for analysing precious samples such as meteorites. This technique is the most powerful method to characterize the nature of carbonaceous matter present in the ordinary chondrite. In the present work, analysis of Dergaon H5 ordinary chondrite (Grossman and Zipfel 2001) using mid-infrared (transmittance) are presented in order to facilitate an understanding of the relative nature of the SiO₄ tetrahedra in 800-1100cm⁻¹ (10 μ m) and 800-400cm⁻¹ (20 μ m) region and characterized aliphatic functional CH₂ and CH₃ groups in the spectral region around 2800-3000 cm⁻¹ (3.4 μ m). Composition is presented with the help of X-ray fluorescence (XRF) spectroscopy.

2. Experimental Method

The sample preparation was performed in ultra-clean conditions. To avoid surface contamination we remove the exterior. We took only pieces coming from its interior. The environmental contamination on the sample was checked by optical microscopy. Sample preparation tools were cleaned with conventional method and the samples were crushed following the standard procedure. The X-ray fluorescence (XRF) data on the Dergaon H5 chondrite were collected by using powdered homogenous sample in pellet form. The XRF study was performed on a Philip Magix XRF spectrometer PRO model PW 2440 in wavelength dispersive mode. Typical uncertainty involved is ± 0.02 wt %. The thin sections of the sample have been characterized by electron microprobe analyzer. The experimental details were same as described elsewhere (Bhandari et al. 2005, Dhingra et al. 2004). We tried to minimize the grinding time to avoid the deformation of the crystal structure, the ion exchange and the water absorption from atmosphere. The iron part of the sample was separated with the help of a strong magnet. The powdered sample was homogenized in spectrophotometric grade KBr (1:20) in an agate mortar and was pressed 3mm pellets with a hand press. The infrared spectra was acquired using Perkin-Elmer system 2000 FTIR spectrophotometer with heliumneon laser as the source reference, at a resolution of 4 cm⁻¹. The spectra were taken in transmission mode in the region 400-4000 cm⁻¹. The room temperature was 29°C during the experiment.

3. Results and Discussions

The elemental composition of Dergaon H5 chondrite was determined by X-ray fluorescence (XRF) using the Dhajala (H3) meteorite as a standard. The classification, petrological and chemical characteristics of the Dergaon H5 chondrite has been reported by Shukla et al (2005). The compositional result of this study shows good agreements with the results of Shukla et al. The values of the major elements of Dergaon H5 chondrite is listed in Table 1(a). The only deviation that is readily evident is the distinctly to the K content compared to the previous workers. The olivine composition of the meteorite is presented in Table 1(b). The fosterite and fayalite compositions are Fo_{80} and $Fa_{19.33}$ respectively. Pyroxene composition of is approximately Enstatite, En_{80} Wo₃ $Fs_{16.9}$.

	Element (wt%)											
Sample	Si	Mg	Ca	A1	Fe	Ni	Mn	Cr	K	Р	Na	Ti
This	17.03	14.26	1.1	1.2	27.73	1.7		0.03	0.067	0.1	0.67	0.0
work			9	0		5				5		4
Shukla	Nd	13.6	1.0	1.0	27.30	1.8	2329	3705	352	Nd	7061	Nd
et al			8	9		2	(ppm)	(ppm)	(ppm)		(ppm)	
(2005)												

Table 1(a). Element composition of Dergaon Meteorite (Nd: Not determined.)

Table 1(b). Olivine composition and major mineral phase of the Dergaon Meteorite

Oxides (wt%)								
Sample	Si02	Cr_2O_3	Fe0	Mn0	MgO	NiO	Ca0	Total
Sample 1	39.030	0.047	18.400	0.455	41.372		0.294	99.568
Sample 2	38.900	0.047	18.734	0.475	41.512			99.668
Sample 3	39.297		18.999	0.465	41.774	0.063	0.261	100.859



08/09/25 13:20 x:1scan, 4.0 cm-1, apod none, smooth

Figure 1. FTIR spectrum of the Dergaon meteorite in between 4000-400 cm⁻¹ contains 10 μ m (800-1150cm⁻¹), 20 μ m (400-700cm⁻¹) and 3.4 μ m (2800-3000 cm⁻¹) band. In 1150-400 cm⁻¹ region, the spectrum exhibits four characteristics bands of olivine. The aliphatic stretching component is represented by the group of peaks in the 3000.2800 cm⁻¹ region.

Table 2. Infrared peak positions in 10µm and 20µm region of Dergaon meteorite and their possible
assignments are presented. Table indicates the four characteristic infrared peak positions of olivine group in
the Dergaon meteorite (Wavenumber in cm ⁻¹). The observed peak positions of Dergaon are compared with
the olivine group i.e. fayalite, forsterite and enstatite according to the infrared data of Gadsden (1975).

Region Fayalite		Forsterite	Enstatite	Dergao	Assignments		
	(Fe_2SiO_4)	(Mg_2SiO_4)	(Mg_2SiO_3)	n			
			1128-04	1126	asymmetric stretching vibration,		
					Si-O(TO2-T2O5)		
	1060	1053	1070-56	1057	asymmetric stretching vibration,		
					Si-O(TO2-T2O5)		
		1000-990	1020-10	1006	asymmetric stretching vibration,		
					Si-O(TO2-T2O5)		
10µm	1012	965-55	965-58	982	Si-O asymmetric vibration, Si-O(TO3)		
	976-82	982	950-47				
	920-35	932	915-20	922	Si-O asymmetric vibration, Si-O(TO3)		
	902-08	886-82	880-73	890	Si-O asymmetrical vibration, (T2O7		
					TO4)		
	852-77				Si-O asymmetrical vibration, (T2O7		
					TO4)		
		840		842			
	828						
			719-28	723	O-Si(Al)-O symmetrical Bending		
20µm			693-95	687	O-Si(Al)-O symmetrical Bending		
		620-02		630-596			
	558-66	545	535	537			
	510-02	512-01	505	507	Si-O and Mg-O vibration		
	480-82	473-63	460	469	Si-O-Si bending vibration		
		430-28		429			

The infrared spectrum as shown in the Figure 1, reveals a number of absorption bands in the 10µm $(800-1150 \text{ cm}^{-1})$ and $20 \text{ um} (400-700 \text{ cm}^{-1})$ and it indicates the presence of silicates in the sample. The comparison of olivine group with (Gadsden 1975) Dergaon H5 ordinary chondrite is presented in the Table 2. The free SiO₄ ion has exhibit four fundamental vibrational modes: a symmetric stretch (v_1) ; a symmetric bend (v_2) ; an asymmetric stretch (v_3) and an asymmetric bend (v_4) . The strong bands in the 10 μ m (800-1150 cm⁻¹) region is identified as Si-O stretching and the bands present in the 20 μ m (400-700 cm⁻¹) region is assigned as Si-O-Si bending vibrations. The bands found in the decreasing intensities in the Si-O stretching region and the Si-O-Si bending vibrations at 1057, 1006, 982, and 507 cm⁻¹ is identical to the bands of fayalite (Fe₂SiO₄) (Fa₁₉₃₃), the bands found at 469, 507, and 1006 cm⁻¹ is identical to the bands of forsterite $(Mg_{2}SiO_{4})$ and the bands found at 507, 537, 723, 982, 1006, 1057 and 1126 cm⁻¹ are identical to the bands of enstatite (Mg₂SiO₃) (Gadsden,1975). The band found at 504 cm⁻¹ can be interpreted as Si-O and Mg-O vibration modes in enstatite (MgSiO₃) with slight shifts in the matrix (Nakamoto 1978). The petrologic type-5 chondrites have two strong peaks at 982cm⁻¹ and 537 cm⁻¹ which may be related to Fe-O and Mg-O stretching modes (Nyquist et al 1971). In the infrared spectrum the Si-O asymmetric stretching vibration (TO2-T2O5) is observed in between the peaks 1006-1126 cm⁻¹. In between the peak position 982 cm⁻¹ and 890 cm⁻¹ we observed the Si-O asymmetric vibration (TO3) and (T2O7- -TO4) respectively. In the bending vibration region, the symmetrical bending vibration of O-Si (Al)-O is observed at the peak position 687 cm⁻¹. Another peak is observed at 469 cm⁻¹ which is due to Si-O-Si bending vibration.

We observed some trace around 3600-3700 cm⁻¹ region which may be due to O-H stretching of structural hydroxyl features of phyllosilicates. Generally OH groups reside at the octahedral surface of the layers and forms weak hydrogen bonds with the oxygen of the Si-O-Si bonds on the lower surface of the octahedral plane (Madejova et al 2001). The presence of very week band at 1650 cm⁻¹ is attributed to H-O-H bending vibration. Another strong peak at 3430 cm⁻¹ is arising due to the dissolved volatile species.

Sample	Peak position	% Transmission	Intensity	Assignments
At room temperature	2954	33.0165	0.48127	CH ₃ stretching vibration
	2923	31.8190	0.49313	CH ₂ stretching vibration
	2842	33.2560	0.47813	CH ₂ symmetric stretch
80°C after 24 hour	2956	12.4985	0.90314	CH ₃ stretching vibration
	2921	12.3628	0.90788	CH ₂ stretching vibration
	2862	12.7698	0.89382	CH ₂ symmetric stretch
80°C after 48 hour	2926	24.9472	0.60298	CH ₂ stretching vibration
	2858	25.8187	0.58807	CH ₂ symmetric stretch

Table 3. Infrared band positions of 3.4 µm region and assignments of the Dergaon meteorite.

In 3.4 μ m (2800 – 3000 cm⁻¹) region three major peaks are found corresponding to aliphatic hydrocarbon stretching features. The pair of peaks at 2922 and 2851 cm⁻¹ corresponds to the asymmetrical and symmetrical stretching vibrations of CH₂ in an aliphatic hydrocarbon. The peaks at 2958 and 2865 cm⁻¹ correspond to the asymmetrical and symmetrical stretching vibrations of CH₃ also in an aliphatic hydrocarbon (Salisbury et al 1992; Socrates 2001; Matrajt et al 2004). The sub-features of both symmetric and asymmetric C–H stretching vibrations of –CH₂– and –CH₃ of aliphatic entitles with C–C single bonds. At room temperature, Dergaon meteorite shows weak absorptions of C-H stretching bends in between 2852–2972 cm⁻¹, indicating polyatomic entitles with C bonded to two or three H. The strongest v _{CH} bend in between 2921–2926 cm⁻¹ assigned to symmetrical stretch of C–H mode of –CH₂– group. The bend in between 2842–2862 cm⁻¹ is assigned to asymmetrical stretch of –CH₂- group. Another bend is found at 2954–2956 cm⁻¹ due to symmetric stretch of –CH₃ group (Table. 3). The variation of the peak intensity in $2800 - 3000 \text{ cm}^{-1}$ region is observed by heating the pellet at a constant temperature 80°C with a time difference of 24 hours. The intensity of the peak shows a discrepancy with time. In the CH₃ stretching vibration around 2954-56 cm⁻¹ significant changes observed after 48 hours (Fig.2 c). On further heating for 24 hours, the bands in this region are disappeared. There is no significance change is observed due to temperature treatment in the Si-O stretching and bending region. The weak absorption bands observed in the Dergaon meteorite are indicative to organic compounds present in the meteorite, the features observed in other H-chondrites by Lawless *et al.* (1972). The stretching features of aliphatic hydrocarbon are generally not observed in the meteorite of H types. The cause of weathering in the studied meteorite sample may be responsible for presence of aliphatic hydrocarbon stretching features. Further work on phase stability of CH stretching region and weathering nature of Dergaon meteorite are under progress.



Figure 2. The infrared spectra in 2800-3000 cm⁻¹region exhibits aliphatic hydrocarbon in Dergaon meteorite. The spectra demonstrate the change of peak positions with temperature. (a) at room temperature (29°C), (b) heating at constant temperature 80°C for 24 hours, (c) heating at constant temperature 80°C for 48 hours, (d) heating at constant temperature 80°C for 72 hours. The spectra show the variation of peak intensities with time.

4. Conclusion

The data obtained during this work characterized the olivine group and aliphatic hydrocarbon (CH₂ and CH₃) in the Dergaon H5 chondrite. Prominent peaks at 1006, 982, 922, and 890cm⁻¹ of infrared spectra correspond to the four characteristics band of olivine group present in the meteorite sample which is originated from the valance vibrations of SiO_4 tetrahedra, a basic component of the silicate lattice. The infrared band observed in the 2842-2962 cm⁻¹ region is indicative to stretching features of aliphatic hydrocarbon. The weathering of the meteorite sample cannot be overlooked for presence of these features. If we ignore the terrestrial and atmospheric contaminations occurred due to sample collection and preservation, the presence of stretching features of aliphatic hydrocarbon is indicative to the organic compounds, which significant for astrobiology.

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