

- and Arnold, J. R., *Proc. Lunar Planet Sci. Conf.*, 1978, 9th, 2299.
9. Venkatesan, T. R., Nautiyal, C. M., Padia, J. T. and Rao, M. N., *Proc. Lunar Planet. Sci. Conf.*, 1980, 11th, 1271.
 10. Goswami, J. N. and Nishiizumi, K., *Workshop on Lunar Breccias and soils and their meteoritic analogs*, 1981, LPI Tech. Report 82-02, 44.
 11. Hohenberg, C. M., Marti, K., Podosek, F. A., Reedy, R. C. and Shirck, J. R., *Proc. Lunar Planet. Sci. Conf.*, 1978, 9th, 2311.
 12. Goswami, J. N., Lal, D. and Wilkening, L. L., *Space Sci. Rev.*, 1984, 37, 111.
 13. Lugmair, G., Marti, K., Kurtz, J. P. and Scheinin, N. B., *Proc. Lunar Sci. Conf.*, 1976, 7th, 2009.
 14. Padia, J. T., Rao, M. N. and Venkatesan, T. R., *Lunar and Planetary Science*, 1985, XVI, 532.

hydrogen bonds made by water II. Adjacent chains are bonded by weaker hydrogen bonds by water I. The factor group analysis predicts 333 (excluding 3 acoustic modes) vibrational modes at $k = 0$.

$$\Gamma_{333} = 42 A_g + 42 B_{1g} + 42 B_{2g} + 42 B_{3g} \\ + 42 A_u^{(o)} + 41 B_{1u} + 41 B_{2u} + 41 B_{3u}$$

The g modes are Raman active and u modes except A_u are infrared active. The highest possible symmetry of HPO_4^{2-} ion (considered as HOPO_3^{2-}) is C_{3v} , corresponding to free rotation of the hydroxyl group about its P-O bond⁵. Of the 12 internal modes of HPO_4^{2-} ion, $9(3A_1 + 3E)$ are associated with PO_4 group and 3 with OH group. These modes are both IR and Raman active.

In the crystal, the HPO_4^{2-} ions occupy sites of lower symmetry than its free ion symmetry (C_{3v}). This leads to anisotropic crystal field which removes the degeneracies of the normal modes. The non-degenerate PO_3 symmetrical stretching mode, correlated to A_1 species of the PO_4^{3-} ion with T_d symmetry splits into two components both in IR and Raman (table 1). The splitting of this nondegenerate mode is due to the resonance interaction between vibrating ions of the unit cell. Two types of HPO_4^{2-} ions producing these two lines are not possible, since no doubling of lines corresponding to other stretching modes is observed. The P-O(H) stretching mode (A_1) and PO_3 asymmetric stretching mode (E) are derived from the triple degenerate P-O asymmetric stretching mode (F_2) of PO_4 group with T_d symmetry. The bands observed due to these modes are strong both in IR and Raman.

In order to assign the deformation vibration of HPO_4^{2-} ion, it has been assumed that the bending modes of HPO_4^{2-} ion consist of $\delta_{as} \text{PO}_3(E)$, $\delta_s \text{PO}_3(A_1)$ and $\delta \text{P(OH)}(E)$ vibrations. Bands due to these modes have appeared in the $390\text{--}600 \text{ cm}^{-1}$ region. The relationship between ν_{OH} and $r(\text{O-H})$ suggests an OH stretching frequency in the $2700\text{--}3000 \text{ cm}^{-1}$ region⁶. The band at 2910 (IR and Raman) has been assigned to (P) O-H stretching mode. The bands at 2440 and 2330 cm^{-1} (IR) are taken as combinations.

The two doublets in the OH stretching region of water indicates two crystallographically distinct types of water molecules in the crystal. The bands corresponding to each water molecule have been assigned on the basis of their hydrogen bond strength. The bands in the $450\text{--}700 \text{ cm}^{-1}$ region have been tentatively assigned to librational modes of water⁷. The OPO bending modes have also been observed in this region.

VIBRATIONAL SPECTRUM OF $\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$

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COMPOUNDS in the series $\text{Na}_2\text{HPO}_4 \cdot n\text{H}_2\text{O}$ ($n = 0, 2, 7, 12$) are of considerable interest and have been the subject of extensive experimental investigations¹⁻⁴. X-ray structural studies of $\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$ have indicated the presence of two distinct types of water molecules and the nature of hydrogen and coordination bonds in the crystal². Chapman and Thirlwell⁴ from their IR analysis showed two distinct HPO_4^{2-} ions in $\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$ contrary to the x-ray results. A vibrational study has been attempted to resolve the ambiguities in the structure and to understand the dynamics of the crystal.

The IR spectrum of the sample prepared as KBr pellet has been recorded on a Perkin-Elmer 283 spectrophotometer. A SPEX Ramalog 1401 equipped with a Spectra Physics model 165 Ar^+ laser (5145 \AA line with $100\text{--}200 \text{ MW}$) has been used to record the spectrum.

$\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$ crystallizes in an orthorhombic system with space group Pbca (D_{2h}^{15}) and has eight molecules in the unit cell². Sodium atoms and HPO_4^{2-} ions are in general positions. The two water molecules occupy crystallographically non-equivalent C_1 sites. HPO_4^{2-} groups are linked into an infinite chain by the

Table 1 Vibrational spectral data and assignments for $\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$

Raman cm^{-1}	IR cm^{-1}	Assignment
3450 m	3440 s	Water I
3375 m	3380 w	ν_{as} Water II
3123 m	3120 m	Water I
3079 m	3080 w	ν_{s} Water II
2910 w	2910 w	(P)O—H stretch
	2440 m	Combinations
	2330 w	
	1710 m	HOH bending
1258 vw	1260 m	Inplane POH bending (β OH)
1143 s	1120 s	PO_3 asy-stretch
1067 s	1055 s	
990 sh	980 sh	PO_3 sym. stretch
952 vs	950 s	
865 s	860 s	P—O(H) stretch
800 vw	810 m	Out of plane POH bending (γ OH)
700 vw	690 w	Rr water
571 s	580 vw	PO_3 asy. bending
544 m	540 w	
	525 w	Rt water
516 s	510 s	PO_3 sym. bending
452 m		Rw water
412 m	385 w	OPO (H) bending
399 s		
350 w		
288 w		$\text{Na}^+ \dots \text{O}$ stretch?
229 w		
195 w		
156 w		Lattice modes
143 w		
104 w		OH \dots O stretch?
96 w		
79 w		

Rw, Rt, Rr: wagging, twisting and rocking libration.
s—Strong, m—medium, w—weak

As the identification of the external modes is difficult without single crystal data, the bands below 350 cm^{-1} have been assigned to the lattice modes. The proposed assignments are given in table 1.

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1. Baur, W. H. and Khan, A. A., *Acta Crystallogr.*, 1970, **B26**, 1584.
2. Catti, M., Ferraris, G. and Franchini Angela, M., *Acta Crystallogr.*, 1977, **B33**, 3449.
3. Catti, M., Ferraris, G. and Ivaldi, G., *Acta Crystallogr.*, 1978, **B34**, 369.
4. Chapman, A. C. and Thirlwell, L. E., *Spectrochim. Acta*, 1964, **20**, 937.
5. Chapman, A. C., Long, D. A. and Jones, D. T. L., *Spectrochim. Acta*, 1965, **21**, 633.

6. Novak, A., *Structure and bonding* (ed.) A. D. Dunitz 1973, Vol. 19, p. 176 (New York: Berlin Heidelberg).
7. Jain, Y. S., *J. Phys. Chem. Solids*, 1976, **37**, 641.

RESULTS OF A MAGNETIC STUDY ON A CHROMITE REEF AT TEKURU IN THE EASTERN GHATS BELT

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IN geophysical literature there are a large number of reports¹⁻⁵ on the exploration for chromites. They include successes, failures and controversies in delineating chromite ore bodies by employing the magnetic method. In this note results of field and laboratory magnetic investigations over a chromite occurrence at Tekuru ($17^\circ 23' \text{ N}$, $81^\circ 35' \text{ E}$) are examined. The chromite ore at Tekuru is associated with ultramafic rocks like chromitites and pyroxenites. The country rocks are the khondalite gneisses. The chromite reef, exposed on the crest of Erukonda hill, strikes at $\text{N}45^\circ \text{ E}$ with a dip of 75° SE . On either side of the crest the reef is covered by thick soil and its width varies around two metres⁶.

Vertical magnetic field observations were made, along lines perpendicular to the strike of the chromite reef at intervals of 3 m in general and near the reef at intervals of 1.5 m. Four such parallel traverses, at an interval of 30 m, were made with a torsion magnetometer (Askania Werke make) which has a scale value of 250 γ s and a reading accuracy of about 2 γ s. The observations were referred to a Base Station for purposes of data reduction and the anomalies are shown plotted in figure 1. The 1800 γ anomaly on profile (1) and -2100γ anomaly on profile (2) were observed on the outcropping khondalite gneisses. A minimum (-250γ s) on profile (4) coincides with the position of the chromite reef. There is a similar low in the strike direction of the reef on profile (3). These are not the only lows on the profiles. So, the anomaly due to chromite is not conspicuous. In the unoccupied portion of profile (1) the area is characterised by a scarp-like sharp descent. Towards NE of profile (4) the area is marked by an increase in elevation and outcropping country rock gneisses. Seven samples of chromite ore and four samples of the khondalite gneiss were collected for the determination of their NRM