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X-ray diffraction study of bituminous coal. By G. B. MITRA, Department of X-rays and Magnetism, Indian Association for the Cultivation of Science, Calcutta 32, India

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With a view to studying the structure of bituminous coal by employing improved and accurate techniques, several Indian samples of vitrain have been examined by the X-ray diffraction method using nickel-filtered Cu  $K\alpha$  radiation. The X-rays were collimated by a cylindrical slit of diameter 0.5 mm. and length 9 cm. and fell upon a sample stick of diameter 0.5 mm. mounted on a goniometer head along the axis of a cylindrical camera of radius 4.66 cm. The direct beam was stopped by a lead shield of diameter 1.0 cm. The intensity distribution in the diffraction photographs was found by means of a microphotometer, using a photomultiplier tube. The photographs obtained (Fig. 1) show (a) a



Fig. 1. Microphotometer records of X-ray diffraction photographs of (a) bituminous coal, (b) carbon black.

comparatively sharp and strong band corresponding to a spacing of 7.11 Å, (b) a very intense and broad band corresponding to a spacing of 4.45 Å, and (c) a diffuse and weak band corresponding to a spacing of 3.6 Å. The last two bands are inseparably joined; together they form a very broad band, indistinguishable but for their difference in intensity.

It is noteworthy that the 2.12 Å weak band reported by previous workers (Mahadevan, 1929; Blayden, Gibson & Riley, 1944) could not be found, even in overexposed films. The spacing of this band corresponds to the (100) line of graphite. This band, together with the 3.6 Å band corresponding to the (002) line of graphite, form the basis of the graphite theory of the structure of coal. The 4.45 Å band has no corresponding line in the powder pattern of graphite and is attributed by Blayden *et al.* (1944) to the bitumen lamellae. The author, however, in the course of these investigations has also observed the 4.45 Å band (together with other bands present in the diffraction photographs of coal) in the diffraction photographs of several samples of carbon black. Also, Gupta (1949) has observed a band of approximate spacing 5 Å in some carbonaceous substances when carbonized under various temperatures and pressures. Thus the 4.45 Å band does not appear to be due to bitumen.

The 7.11 Å band has not been reported before, although Turner & Anderson (1931) observed a 6.53 Å band in a Pennsylvania anthracite and interpreted it as representing the average distance between a carbon layer in a particle and the corresponding carbon layer in the next particle. Such an explanation for the 7.11 Å band would require this band to be very diffuse, at least more diffuse than the 3.6 Å band. The microphotometer curves, however, show the 7.11 Å band to be fairly sharp and definitely sharper than the 3.6 Å band. Also, the above picture presumes a preferred arrangement of particles which is extremely unlikely in artificial amorphous carbon such as carbon black. However, the carbon blacks examined give diffraction photographs showing this 7.11 Å band along with the other bands found in coal. Thus, this theory of interparticle arrangement is untenable.

As both the Bernal (1924) and Lipson & Stokes (1942) structures of graphite are unable to explain the origin of this band, further studies are being carried out to elucidate the structure of carbon in coal. A more detailed report will be published shortly.

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## References

- BERNAL, J. D. (1924). Proc. Roy. Soc. A, 106, 749.
- BLAYDEN, H. E., GIBSON, J. & RILEY, H. L. (1944). Proceedings of a Conference on Ultrafine Structure of Coals, p. 176. Edited by D. H. Bangham and D. P. Riley. London: The British Coal Utilization Research Association.
- GUPTA, N. N. (1949). J. Sci. Industr. Res. B, 8, 238.
- LIPSON, H. & STOKES, A. R. (1942). Proc. Roy. Soc. A, 181, 101.
- MAHADEVAN, C. (1929). Ind. J. Phys. 4, 79.
- TURNER, H. G. & ANDERSON, H. V. (1931). Industr. Engng. Chem. 23, 811.